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DESCRIPTION

THREE-DIMENSIONAL STRUCTURE OF LIPOCALIN-TYPE PROSTAGLANDIN

D SYNTHASE AND UTILIZATION OF THE SAME

5 TECHNICAL FIELD

The present invention relates to the three dimensional structure of lipocalin-type prostaglandin D synthase (may be referred to as "L-PGDS" hereinafter). The present invention also relates to a method for selecting an inhibitor of L-PGDS using the three dimensional structure.

BACKGROUND ART

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Prostaglandin (PG) D_2 is actively produced in various tissues and involved in many physiological phenomena. In central nervous system, PGD_2 accelerates non-rapid eye movement (NONREM) sleep and regulates nociceptive reaction. PGD_2 is also actively produced by mast cell, basophil, and T helper type-2 cell, and controls allergy reaction via DP and CRTH2 receptors. PGD_2 is converted to J series of prostaglandin such as 9α , 11β - PGF_2 and PGJ_2 , Δ^{12} - PGJ_2 , and 15-deoxy- $\Delta^{12,14}$ - PGJ_2 . These prostaglandins have quite different properties in biological system. 15-Deoxy- $\Delta^{12,14}$ - PGJ_2 acts as a ligand of PPAR γ , i.e., nuclear receptor involved in the differentiation of adipocyte, macrophage, and monocyte, preventing NF- κ B and AP-1 dependent gene

expression.

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Arachidonate cascade starts from PGH₂ synthase (cyclooxygenase, COX) and the enzyme produces PGH₂ from arachidonic acid provided from lipid bilayer of cell membrane. PGH₂ having 9,11-endoperoxide is unstable and spontaneously decomposes to be isomerized mainly to PGE₂ having 9-keto and 11-hydroxy group. PGD₂ having 9-hydroxy and 11-keto group is a redio isomer of PGE₂, and is specifically produced from PGH₂ by PGD syntase (PGDS, Prostaglandin H₂ D-isomerase [EC5.3.99.2]).

There are two types of PGDSs genetically different One is hemopoietic enzyme (hemopoietic from each other. PGD Synthase; H-PGDS) and the other is lipokalin-type enzyme (lipokalin-type PGD Synthase; L-PGDS) (Y. Urade and O. Hayaishi, Vitamins Hormones 58:89-120 (2000)). H-PGDS has molecular weight of 26 KDa and is a glutathione-dependent It is mainly localized in antigen-presenting cell mast cell. H-PGDS belongs to sigma class and glutathione S transferase (GST) as assessed by evolutional and crystallographic analysis. On the other hand, L-PGDS has molecular weight of 26 KDa, which is identical with that of H-PGDS, but is glutathione-independent enzyme and quite differs from H-PGDS in amino acid sequence, gene structure, evolutional origin and cellular localization.

L-PGDS is a member of a lipokalin gene family composed

of various secretory proteins and localized in choroid plexus, arachnoid membrane, and oligodendroglia of central nervous system (Y. Urade and O. Hayaishi, Biochem. Biophys. Acta, 1482:259-271(2000)). L-PGDS gene knock out mice lack allodynia induced by γ -aminobutyric acid and touch-evoked 5 pain (Eguchi et al., Proc. Natl. Acad. Sci. USA, 96:726-730 (1998)), and have small NONREM sleep rebound after sleep al., The 3rd deprivation (Eguchi et International Conference on Oxygen and Life, Kyoto, Vol. 1233C:429-433(2002)). Megalocardia induced by loading high fat food 10 1ow knockout mice. is in the gene Human L-PGDS overexpressing mice exhibit an excessive amount of NONREM the algetic stimulation, which occurs sleep after simultaneously with the increase of PGD2 in brain (Pinzar et al., Proc. Natl. Acad. Sci. USA, 97:4903-4907(2000)). 15 L-PGDS is considered to contribute to the control of algetic appearance and NONREM sleep by producing PGD2 in central nervous system. In addition, allergic airway inflammation is exalted in human L-PGDS overexpressing 20 mouse (Fujitani et al., J. Immunol, 168:443-449(2002)). The exaltation of L-PGDS gene expression is observed in the brain of patients with neurodegenerative disease such as multiple sclerosis (Chabas et al., Science, 294:1731-1735(2001), Thaisacks disease, and Sandhoff disease 25 (Myerowitz et al., Hum. Mol. Genet, 11:1343-1350 (2002))).

The expression of L-PGDS is observed in arteriosclerosis plaque of coronary artery in stable angina pectoris disease (Eguchi et al., Proc. Natl. Acad. Sci. USA, 94:14689-14694(1997)).

Therefore, If an inhibitor of L-PGDS can be found, the inhibitor can be expected to be used as new types of medicines such as allodynia, sleep controlling agent, antiallergic agent, anti-neurodegenerative agent, anti-arteriosclecrosis agent and anti-megalocardia agent.

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DISCLOSURE OF INVENTION

The present invention has an object to clarify three-dimensional structure of L-PGDS and to provide a method for designing and seeking an inhibitor of L-PGDS using the three-dimensional structure.

The present invention provides a crystal of lipocalinderived prostaglandin D synthase from mouse. Lipocalin-type prostaglandin D synthase derived from mouse has an amino acid sequence of SEQ ID NO:1. Since amino acids from sites 1 to 24 are a signal sequence, it is preferred that the protein excluding this portion is used. In addition, mouse L-PGDS contains three cystein residues at sites 65, 89, and 186. Accordingly, it is preferred for resolving crystal structure that, when L-PGDS is produced by recombinant method, cystein at site 65 is replaced by alanine to avoid the formation of disulfide bond other than native disulfide bond between cystein at sites 89 and 186. L-PGDS in which such substitution is made and the signal peptide is excluded may refer to as "native-type Cys⁶⁵Ala L-PGDS" or merely as "native-type L-PGDS" hereinafter.

This native-type L-PGDS crystal has a space group $P2_12_12_1$ of orthorhombic system and the size of unit cell is $a=46.2\pm0.5\text{\AA}$, $b=66.8\pm0.7\text{\AA}$, and $c=105.3\pm1.0\text{\AA}$. There are two molecules of L-PGDS in crystallographic asymmetric unit.

Another crystal is produced from L-PGDS in which methionine at sites 64, 94, and 145 are replaced by seleno methionine in addition to exclusion of signal peptide and Cys⁶⁵Ala substitution (may refer to as "Se-Met-type L-PGDS" hereinafter).

This Se-Met-type L-PGDS crystal has a space group $C222_1$ of orthorhombic system and the size of unit cell is $a=45.7\pm0.5\,\text{Å}$, $b=66.8\pm0.7\,\text{Å}$, and $c=104.5\pm1.0\,\text{Å}$. There is one molecule of L-PGDS in crystallographic asymmetric unit.

The present invention is related to lipocalin-type prostaglandin D synthase having the three-dimensional structure represented by the structure coordinates of Table

2. The structure coordinates were

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obtained by X-ray structure analysis of "native-type L-PGDS" as described above.

25 The present invention is related to lipocalin-type

prostaglandin D synthase having the three-dimensional structure represented by the structure coordinates of Table 3. The structure coordinates were obtained by X-ray structure analysis of "Se-Met-type L-PGDS" as described above.

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Crystal structures of native-type Cys⁶⁵Ala L-PGDS and Se-Met-type L-PGDS are presumed to be identical with wild type L-PGDS by the following reasons:

- (i) The catalytic mechanism of PGDS reaction can be reasonably explained by the crystal structure of native-type Cys⁶⁵Ala L-PGDS;
- (ii) As apparent from the interaction with PGH₂, the side chain of cystein residue at site 65 is exposed to the surface of inner cavity of the protein, and is not involved in the formation of disulfide bond which is an element of the protein skeleton in wild type L-PGDS having PGDS activity;
- (iii) The fact that even Cys^{89,189}Ala variant not having disulfide bond of protein skeleton has enzyme activity which is a phenotype of the structure suggests that the barrel structure of L-PGDS itself is strong, and that the structure of native-type Cys⁶⁵Ala L-PGDS is not significantly changed by the amino acid substitution;
- (iv) The three dimensional structure of Se-Met-type L-PGDS is very similar with that of native-type Cys⁶⁵Ala L-

PGDS.

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and 3 represent the three-dimensional structure coordinates according to the format of Protein Data Bank (http://rcsb. org/pdb/, USA). "ATOM" first column indicates that it is atom constituting protein; the second column indicates the atom number from first sequentially numbered the amino constituting the protein; the third column indicates the atom type constituting the protein. For example, $C\alpha$ carbon atom is represented by CA; amido nitrogen atom represented by N; carbonyl carbon atom is represented by C; and carbonyl oxygen atom is represented by O,; the fourth column indicates the amino acid residue by three letter notation; the fifth column indicates the class of molecule; the sixth column indicates the amino acid number; the seventh, eighth, and ninth columns indicate coordinates of the atom (in A for X-axis, Y-axis, and Z-axis directions in the order); the tenth column indicates the occupancy of the atom (in the present invention 1.00 for all atoms); and the eleventh column indicates the temperature factor of the The twelfth column indicates the class of atom in atom. Table 2 and the class of molecule in Table 3.

When these coordinates are used, an inhibitor of L-PGDS can be selected. That is, the present invention is related to the use of the coordinates described in Table 2

or 3 for the selection of lipocalin-type prostaglandin D synthase inhibitor.

The present invention relates to a method for selecting an inhibitor of lipocalin-type prostaglandin D synthase, which comprising:

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- (a) providing the three dimensional coordinates of Table 2 or 3 representing the three dimensional structure of lipocalin-type prostaglandin D synthase:
- (b) providing three dimensional structures of candidate compounds; and
 - (c) selecting the candidate compound which fits to the substrate-binding site of lipocalin-type prostaglandin D synthase.

The term "substrate-binding site of L-PGDS is an interior space of hollow structure determined by amino acids residues at sites 39, 43-48, 54, 65-67, 77-83, 90-96, 103-107, 116-120, 129-133, 143-149 and 180 in amino acid sequence of L-PGDS of SEQ ID NO:1. These regions include 1 to 5 amino acids before and after the amino acid residues.

The term "fit" means that the whole or the part of candidate compound can stably bind to the whole or the part of the above substrate-binding site in figure and energy. As the result, the binding of the substratre to L-PGDS is inhibited.

In a preferred embodiment, the inhibitor as selected

above is contacted with L-PGDS in the presence of prostaglandin H_2 to measure L-PGDS enzyme activity to confirm the inhibiting effect of the inhibitor selected.

According to the method of the present invention, a novel inhibitor of L-PGDS was found. That is, the present invention relates to an inhibitor of lipocalin-type prostaglandin D synthase, 4-dibenzo(a,d)cyclohepten-5-ylidene-1-(4-(2H-tetrazole-5-yl)butyl)piperidine (referred to as "AT-56" hereinafter).

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BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows the whole structure of L-PGDS.

- (A) is ribbon diagram of $P2_12_12_1$ crystal of native-type L-PGDS which are viewed from right angle to barrel. The upper is open terminus of the barrel and the lower is closed terminus. Strands and helixes are represented as A-H and 1-3, respectively.
- (B) is a drawing showing the electrostatic feature of L-PGDS viewed from open (referred to as "o") and closed (referred to as "c") terminus. Black is electrostaticly positive and white, negative.
- (C) is a drawing showing conserved surface of L-PGDS. The degree of amino acid sequence conservation of known L-PGDS is depicted on the L-PGDS molecule surface. Dark shows higher conservation.

Figure 2 is a sequence alignment in consideration of mouse L-PGDS and other lipocalin structure. SCR region in which high amino acid conservation is observed in all sequences constitute the closed terminus of the barrel structure, and presumed to be important for L-PGDS activity. L-PGDS has a signal sequence consisting of about 20 residues at N-terminus region.

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PGDS: mouse L-PGDS, HNGAL: human neutrophils gelatinase related lipocalin, BLG: human β -lactoglobulin, RBP: human retinol binding protein, ERABP: rat epididymis retinoic acid binding protein, MUP: mouse main urine protein, OBP: ox perfume substance binding protein, BBP: butterfly biline binding protein.

Figure 3 shows characteristic features of L-PGDS structure.

- (A) is a stereo diagram of the whole skeleton structure of L-PGDS of Se-Met type C222₁ crystal having noteworthy feature. Eight residues in hydrophilic belt inside envelop are shown. The structure in which one S-S bridge of Cys89/186 and two aromatic residues Trp⁵⁴ and His ¹¹¹ are contacted is found in the upper end of the barrel structure. Gln⁵¹ at upper left and Gln⁷⁸ at lower light are two presumed glycosylated sites.
- (B) is a closed-up of hydrophilic belt. There are eight polar residues, $Cys^{65}Ala$, Ser^{45} , Thr^{67} , Ser^{81} , Tyr^{149} ,

Thr 147 , Ser 133 , and His 116 , which form presumed binding-site of the substrate-binding site of PGH $_2$.

Figure 4(A) shows a stereo diagram showing closed and open manner of envelop entrance. His 111 of EF loop can closes (H111c) or open (H111o) the entry of the substratebinding site by the aromatic interaction of Trp54 of Ω loop.

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(B) is a stereo diagram of the bottom of substrate-binding site around Phe^{39} and Trp^{43} . Two rotational isomer are shown in $P2_12_12_1$ (F390) and $C222_1$ (F390) crystal structure.

Figure 5 is a stereo diagram showing suggested PGH_2 bonding manner of L-PGDS. The PGDS binding and the presumed residue thereof involved in catalyst are shown with PGH_2 bonded.

Figure 6 is a schematic view of reaction mechanism. Hydrogen bond net work including Cys⁶⁵ promotes the formation of thiolate anion at physiological pH by sifting thiol and thiolate. After the binding of PGH₂ (1), thiolate of Cys⁶⁵ attacks as base endoepoxyoxygen attaching to C11 atom (2) to form S-O adduct as an intermediate(3). The unstable S-O bond is cleaved by synergistic rearrangement (3) to form C11 carbonyl of the product PGD₂(4).

Figure 7 is a graph showing binding and dissociating

rate in the binding of PGD_2 , PGE_2 and $PGF_{2\alpha}$ to L-PGDS. The binding of PGD_2 , PGE_2 and $PGF_{2\alpha}$ to L-PGDS were measured by surface plasmon resonance method. The concentration of PGD_2 ranges 0.0 to 7.5 μ M and the concentration of PGE_2 and $PGF_{2\alpha}$ are $10 \, \mu$ M.

Figure 8 is a graph showing the result of measurement of PGDS activity of various protein mutants at pH 8.0, 9.0 and 10.0.

Figure 9 is a ribbon diagram showing L-PGDS to which 10 AT-56 binds.

Figure 10 is a graph showing the inhibition effect of AT-56 on L-PGDS enzyme activity.

Figure 11 is a graph showing the inhibition effect of AT-56 on PGD_2 production.

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Best Mode for Carrying Out the Invention

- (I) Three Dimensional Structure, Substrate-Binding Site and Reaction Mechanism of L-PGDS
- (i) Whole Three Dimensional Structure of L-PGDS

The crystal structure of L-PGDS shows typical folding structure of lipocaline, and comprises anti-parallel β barrel of eight strands, three α helix regions and cterminus strand (Figure 1A). The barrel has a size of $40 \times 30 \times 35$ Å and the strands are cross-linked via conserved disulfide linkage of Cys^{89/186} at the outside of cup-formed

portion. The outer surface of the protein comprises charged or polar amino acid residues. The molecular surface of the presumed entry for ligand is electrostatically positive and can draw the enzyme substrate PGH₂ and the product PGD which are negatively charged.

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The amino acid sequence of L-PGDS is subjected to alinnment with amino acid sequence of various known lipocalins in consideration of the three dimensional structure (Figure 2). L-PGDS is classified as a karnel type lipocalin and has three structurally conserved region (SCR) 1, 2, and 3. These SCRs constitute closed end of the barrel of L-PGDS molecule and consists of N-terminus helix 1, strand A, strands F and G, and strand H. The helix 1 is positioned near the closed end of the barrel and is considered to stabilize the barrel structure by hydrophobic interaction. SCR is conserved even on the L-PGDS molecule surface (Figure 1C). EF loop and Ω loop corresponding to loop AB containing short helix 2 construct the closed cover of the barrel. Two glycosylated sites are positioned at Asn⁵¹ of large cover of Ω loop of L-PGDS and at Asn⁷⁸ of strand C (Arrow in Figure 3A)

In the inside of L-PGDS controlled by hydrophobic side chain there is a remarkable hydrophilic belt consisting of eight polar residues of $Cys^{65}Ala$, Ser^{81} , Thr^{67} , Ser^{45} , Tyr^{149} Thr^{147} , Ser^{133} , and His^{116} from the right to the left in

Figure 5 and Figure 3B. The residues in the polar belt are involved not only in the binding of the substrate PGH_2 but also in the release of the product PGD_2 . As shown by site-directed mutagenesis hereinafter, the release of the product PGD_2 is promoted by decreasing the cost for hydration and dehydration of the polar hydroxyl group of ω chain.

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The presumed catalyst residue Cys^{65} , which is replaced by alanine in the crystal structure, is positioned

10 at the N-terminus of β strand B and faced to the inside of the barrel of open edge of the protein (Figures 5 and 3B). The $\operatorname{Cys}^{65}\operatorname{Ala}$ residue is surrounded by the hydroxyl side chain cluster of Ser^{45} , Thr^{67} , and Ser^{81} within a distance of hydrogen bonding (Figures 3B). These residues form a hydrogen bond net work in the hydrophobic barrel together with Tyr^{149} , Thr^{147} and Ser^{133} .

(ii)Open-Close Conformation Isomer of L-PGDS

We determined two types of crystal structure having open and closed types at the entry of the substrate-binding site of L-PGDS. In Se-Met type L-PGDS crystal structure having space group C222₁, the active site is separated from the outside of the protein by a closed aromatic bridge between ${\rm Trp}^{54}$ of Ω loop and ${\rm His}^{111}$ of EF loop. In native-type L-PGDS crystal having different space group ${\rm P2}_1{\rm 2}_1{\rm 2}_1$, the entry of the substrate-binding site is opened due to

different conformation of EF loop having His¹¹¹ (Figure 4A). Trp⁵⁴ and ¹⁰⁹SPHXGS residues of mobile EF loop are conserved in all identified amino acid sequence of L-PGDS including Xenopus homolog. One of the two molecules of nature type-L-PGDS contained by asymmetric unit of P2₁2₁2₁ crystal is low in electron density corresponding to Pro¹¹⁰, His¹¹¹. Atom model is not applied to electro density for the two residues. It is considered that open-closed conformation isomer of flexible loop play an important role in the binding of substrate and non-substrate ligand to the substrate-binding site of L-PGDS.

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(iii) Lipophilic Retinoic Acid Binding of L-PGDS as Lipocalin

L-PGDS was crystallized in the presence of retinoic acid as an essential crystallizing adjunct. L-PGDS binds to retinoic acid and retinal like many other lipocalins. Phe³⁹ at bottom of the pocket shows the different rotational isomer in different crystal forms $P2_12_12_1$ and C222₁ (Figure 4B). Native type P2₁2₁2₁ crystal has bulky and wide cavity with high residual electron density near Phe³⁹. On the other hand, in Se-Met C222₁ crystal, corresponding residual electron density is continuous with that of Phe³⁹ side chain and a narrower cavity is formed than that of the native type. It is concluded that the residual electron density in the neighborhood of indole

ring of Trp⁴³ near Phe³⁹ side chain in the native crystal is contributed to boundd retinoic acid molecule. These retinoids non-competitively inhibit L-PGDS activity. The binding of retinoids requires the re-organization of hydrophobic residue cluster of L-PGDS including Trp43 which interact with retinoids

(iv) Binding Mode of Substrate PGH2

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When minimum energy PGH2 model is used, the substrate PGH2 is positioned along hydrophilic belt of substratebinding site of L-PGDS (Figure 5). In the suggested binding model, ω chain having 15-hydroxyl group of PGH₂ is inserted into the substrate-binding site, and oxygen atom bound to C11 in endoperoxide bound to cyclopentane ring reaches thiol group of Cys⁶⁵ residue of the catalyst. negative charge of carboxyl group at α chain terminus of PGH_2 is counterbalanced by the positive charge of Lys 92 and Arg85 side chains, which form electrostaticlly positive cover of cup-form portion in a complex model (Figure 5). The hydrophilic belt of the substrate-binding site can promote insertion or release of ω chain of PGH₂ or PGD₂ having polar hydroxyl group since hydrated water of 15 hydroxyl of ω chain in solvent can be exchanged to these side chain without enthalpical dehydration cost. The polar surface of endoperoxide of PGH2 is faced on hydroxyl cluster including Cys⁶⁵ and Ser⁴⁵, Thr⁶⁷ and Ser⁸¹.

hydrophobic portion of cyclopentane structure is enwrapped by hydrophobic chain including Phe⁸³ and Met⁹⁴. The closed conformation of the flexible EF loop existing at the entry of the substrate-binding site provides catalytic space for PGDS reaction and can help to specifically produce PGD₂ by separating catalytic portion from base in solvent. Furthermore, there is space enough to accommodate bulky product PGD₂ having 9-hydroxyl-11-keto-cyclopentan formed in docking study.

10 (v) Reaction Mechanism of L-PGDS

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Reaction mechanism of PGDS activity catalyzed by L-PGDS was presumed and shown in Figure 6. The catalytic residue of L-PGDS is Cys⁶⁵ and the thiol group thereof is reaction species thiolate ion as stabilized as synergistic hydrogen bond network with Ser45, Thr67 and Ser81. Binding mode of PGH2 to L-PGDS in the suggested reaction mechanism provides appropriate configuration to direct endoperoxide oxygen of C11 of PGH2 to sulfur atom of Cys⁶⁵ in PGDS reaction. In the model, the hydrogen-bond network of Cys^{65} with Ser^{45} , Thr^{67} and Ser^{81} decreases pKa of Cys^{65} thiol group and stabilize thiolate anion as species of PGDS catalyst at physiological pH. reaction mechanism is as follows (Figures 6):

Thiolate anion of Cys^{65} attacks endoperoxide oxygen of C11 of PGH_2 as a base (Step 2 in Figure 6) to form S-O

adduct presumed as an intermediate (Step 3). Hydroxyl group of Ser^{45} attacks unstable S-O bond to rearrange proton of C11 hydrogen atom to convert into carbonyl group in a synergistic manner (Steps 3 and 4). After the product PGD_2 is released, thiol proton of Cys^{65} is dissociated to regenerate thiolate anion as reaction species

(vi) Mutant Analysis of L-PGDS

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In order to confirm the suggested substrate-binding and reaction mechanism, site-directed mutagenesis of 9 amino acid residue in the interior of the substrate-binding pocket was performed. Since the preparation of recombinant protein having the same PGDS activity as purified wild-type enzyme is easy, Cys^{89,186}Ala construct was used for this purpose. Various mutants were expressed, purified to homogeneity and L-PGDS activities were compared at pH 8, 9 and 10 (Figure 8).

It was confirmed that Cys^{65} is the catalyst residue of L-PGDS since $\mathrm{Cys}^{65}\mathrm{Ala}$ mutant completely loses enzyme activity. When Ser^{45} , Thr^{67} and Ser^{81} of hydroxyl cluster surrounding Cys^{65} in the catalyst pocket are replaced with Ala, the PGDS activity decreases to 30 to 15 % without significant reduction of Km for PGH₂ (Figure 8 and Table 1). Accordingly, kcat/Km was $0.36\,\mu\,\mathrm{M}^{-1}\mathrm{min}^{-1}$ for $\mathrm{Ser}^{45}\mathrm{Ala}$ and $0.50\,\mu\,\mathrm{M}^{-1}\mathrm{min}^{-1}$ for $\mathrm{Ser}^{81}\mathrm{Ala}$, and thus decreased to one fifth in relative to wild type enzyme. L-PGDS activity is decreased

to less than 10 % of wild type enzyme in Ser^{45,81}Ala double mutant, and almost disappear in Ser⁴⁵, Thr ⁶⁷ and Ser⁸¹ triple mutant. These results correspond to the idea that thiolate anion of Cys⁶⁵ is stabilized by the hydroxyl cluster of Ser⁴⁵, Thr⁶⁷ and Ser⁸¹ to act as a reaction species in the enzyme reaction.

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Notably, three mutants $Phe^{83}Ile$, $Arg^{85}Glu$ and $Lys^{92}Glu$ have kcat/Km of 4.47, 4.86 and $5.71 \,\mu\,\text{M}^{-1}\text{min}^{-1}$, respectively. These values were twice to that of wild type enzyme having kcat/Km of $2.38 \mu \text{ M}^{-1}\text{min}^{-1}$ (Figure 8 and Table 1). On the other hand, Km values of these mutants (11 to $15\,\mu\,\mathrm{M}$ at pH 8) are comparable to wild type enzyme (13 μ M) except for $Arg^{85}Glu$ mutant (7 μ M). These results suggest that the rate-determining step of L-PGDS is not the catalytic process of isomerization, but the product release process. Positive charges of Arg⁸⁵ and Lys⁹² giving positive electrostatic features on ligand entry surface of L-PGDS generate high affinity to negative charge of α chain of PGH₂ and PGD₂ (Figures 1B) and can assist to maintain the product on substrate-binding site. Aromatic ring of Phe85 can assist to accommodare the product in a broad cavity around catalytic Cys⁶⁵ residue as PGH₂ binding model shown in figure 5. The activity of Thr 147 Ala and Tyr 149 Phe mutants decreases to one half in relative to the wild type enzyme. Accordingly, these polar side chains of Thr147 and Tyr149 are important for turnover of the catalyst.

Table 1

Kinetic Parameters of L-PGDS Mutants for PGDS Activity

		Km (μ M)	$Kcat/Km(\mu M^{-1}Min^{-1})$
5	Wild Type(C65)	13	2.38
	S45A	11	0.36
	S81A	12	0.50
	F83I	15	4.47
	R85E	7	4.86
10	K92E	14	5.71
	T147A	19	0.95
	<u>Y149F</u>	1	0.82

^{*}kinetic parameter were measured at pH=8.0

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15 (vii) High Affinity Binding of Product PGD₂ to L-PGDS

L-PGDS binds the product PGD_2 in high affinity $(Kd=89.4\pm3.4\text{nM},\ k_{on}=1.24\text{x}10^3\pm37\text{M}^{-1}\text{sec}^{-1},\ k_{off}=1.11\text{x}10^4\pm7.0\text{x}10^{-6}\text{sec}^{-1})$, Neither PGE_2 nor $PGF_{2\alpha}$ is bound to L-PGDS as measured by surface plasmon resonance analysis (Figures 7) (Jonson et al., Biotechniques 1991 Nov 11 (5):620-627; Beuckmann et al., Biochemistry, 38:8006-8013 (1996)). L-PGDS can act as a PGD_2 transporter protein. Binding and dissociating test show that the bound PGD_2 is slowly released from hydrophobic pocket of L-PGDS. On the other hand, H-PGDS does not show high affinity to PGD_2 . These

results suggest that L-PGDS has two functions. That is, L-PGDS act as a PGD $_2$ synthesis enzyme coupled with COX in cells and thereafter as an extracellular transporter of PGD $_2$.

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(II) Selection of L-PGDS Inhibitor Using Structure Coordinate

It is possible to select compounds which can inhibit L-PGDS using the three dimensional structure coordinates as shown in Table 2 or 3.

The present invention relates to a method for selecting an inhibitor of lipocalin-type prostaglandin D synthase, which comprising

- (a) providing the three dimensional structure coordinates in Table 2 or 3 representing the three dimensional structure of lipocalin-type prostaglandin D synthase:
- (b) providing three dimensional structures of a candidate compounds; and
- 20 (c) selecting a candidate compound which fits to the substrate-binding site of lipocalin-type prostaglandin D synthase.

As described above, the amino acid residues constituting the substrate-binding site of L-PGDS are those at sites 39, 43-48, 54, 65-67, 77-83, 90-96, 103-107, 116-

120, 129-133, 143-149 and 180 in L-PGDS amino acid sequence of SEO ID NO:1.

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Based on the three-dimensional structure information, each candidate compound is evaluated for binding fitness to the substrate-binding site of L-PGDS. In the evaluation, candidate compound and the structure exhibiting stable binding manner in energy and steric structure to the active site of L-PGDS are ranked among candidate compounds having various structures. This evaluation can be automatically performed by many kinds of virtual screening program. Among the ranked candidate compounds, a lead compound is selected which readily bind to the substrate-binding site of L-PGDS numerically and visually. The compound thus obtained is used as basic skeleton, and the derivative capable of binding more stably to the substrate binding site of L-PGDS can be designed and synthesized to develop new inhibitors of the enzyme.

It is preferred to design inhibitor using computer. For example, OCTANE, a workstation supplied by Silicon Graphics, Inc., is suitable as a computer used for designing inhibitors. However, the computer is not limited to this one, and any computer may be used so long as it is tuned to run an appropriate program. Likewise, there is no particular limitation on the computer storage medium. For example, Insight II, a computer program commercially

available from Accelrys, Inc. may be used as a program for designing. In particular, a program Ludi or DOCK, a module of Insight II specially prepared for such purposes, may be used alone or in combination to facilitate identification, searching, evaluation, or designing.

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In designing of inhibitor, there are conceptually two steps. The first step is to find a compound which serves as a starting point for drug design, known for those skilled in the art as a lead compound. The next step is optimization of the lead compound wherein compounds having better properties as medicines, for example, having better activity, having better pharmacokinetics, or having less toxicities and side effects are sought starting from the lead compound.

The step in which a lead compound is found using the structure coordinates of the L-PGDS complex provided by the invention is achieved, present for example, database in a computer into which structures of plural been entered, compounds have by a method in which interactions between three-dimensional structures compound in the database and L-PGDS are sorted out in a visual manner one after another, or by a method in which amplitudes of binding energy are calculated one after another using a computer and compounds which stably bind to PGDS are found from the database. Although it is preferred that the database of compound's structures contains determined three-dimensional structure coordinates entered therein, for low molecular weight compounds, it does not have to be a database of three-dimensional structure coordinates, because such low molecular weight compounds may change their conformations relatively freely, and also because three-dimensional structure coordinates for each conformation can be derived by calculations in a relatively short time. In the latter cases, information for chemical covalent bonds of low molecular weight compounds are entered into the database.

Specifically, in the visual method, L-PGDS is firstly displayed on a computer screen according to the structure coordinates of the present invention. In this step, although a three-dimensional representation may be made on the computer screen using, for example, Crystal Eye as described above, visual examinations can also be achieved without using such a three-dimensional representation.

Chemical interactions to be considered include electrostatic interaction, hydrophobic interaction, hydrogen bonding, van der Waals interaction, and the like. Thus, the structure should be comprehensively examined whether it is favorable for interactions, for example, so that functional groups which tend to bear negative charge such as carboxyl group, nitro group, and halogens interact

with amino acid residues in L-PGDS having positive charge such as lysine, arginine, and histidine, so that functional groups which tend to bear positive charge such as amino, guanidyl groups interact with amino imino, and residues in PGDS having negative charge such as glutamic acid and aspartic acid, so that hydrophobic functional groups such as aliphatic groups and aromatic groups interact with hydrophobic amino acid residues such as isoleucine, leucine, valine, proline, alanine. methionine, phenylalanine, tryptophan and that functional groups involved in hydrogen bonding such as hydroxyl and amide groups can form hydrogen bonds with backbone or side chain portions of L-PGDS, so that binding between the compound and L-PGDS causes no steric hindrance, and so that empty spaces are filled to minimize such empty spaces and maximize van der Waals interaction. Thus, electrostatic interaction, hydrophobic interaction, van der Waals interaction, hydrogen bonding, and other factors are visually and comprehensively considered to determine whether or not the compound is suitable as a lead compound.

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In the method by energy evaluation with a computer, the energy of binding between a compound and L-PGDS is determined by molecular force field calculations. Such calculations are applied to each compound in the database

to find a certain compound which may serve as a lead compound capable of stable binding. As a molecular force field used in the calculations, for example, CVFF, AMBER force field optimized for proteins, which is contained in DISCOVER module of Insight II program may be used. In addition, some computer programs like Ludi in Insight II can automatically output candidates for lead compound when three-dimensional structure coordinates of interacting amino acid residues in a protein molecule are given, and such programs may also be applied to the method of present invention.

Furthermore, the visual examinations and the examination considering energy are not strictly sorted out from each other, and both techniques may be used in combination as appropriate.

The next step, in which optimization of the lead compound is conducted using the structure coordinates of the PGDS complex is used for the purpose of, where a lead compound which binds to L-PGDS has already been found by the above method or separately found in an experimental manner, optimizing the lead compound to obtain a better compound, for example, a compound having higher biological activities as an inhibitor or a compound having a structure favorable for oral administration as a medicine. It becomes possible only after a precise picture of chemical

bonding between the lead compound and L-PGDS has been elucidated to directly find a site which is not optimal for interactions between the lead compound and L-PGDS and to design a new compound having an optimal functional group at that site, thereby enabling to design a more optimized compound.

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For visual examinations with a computer, a model of the complex between the lead compound and L-PGDS is firstly displayed on a computer screen by entering the threedimensional structure coordinates of the lead compound and the structure coordinates of L-PGDS provided by the present invention into a computer on which a computer program expressing three-dimensional coordinates of molecules runs In this step, or into a storage medium of the computer. although a three-dimensional representation may be made on the computer screen using, for example, Crystal Eye as described above, visual examinations can also be achieved without using such a three-dimensional representation. is a logical designing of a compound to modify the lead to yield a compound more favorably as interacting with L-PGDS or a compound having better pharmacokinetics while retaining the interactions.

Chemical interactions to be considered are the same as those in the step to find a lead compound, and a new compound having better properties as an inhibitor is

finally designed starting from the lead compound.

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In the method by energy evaluation with a computer, the energy of binding between a new compound designed from the lead compound and L-PGDS is determined by molecular force field calculations to judge the validity of the design. In addition, it is also possible to use a method in which other molecules such as solvent molecules are additionally included in the model and the free energy is determined using molecular dynamics to derive a compound capable of stable binding. As a molecular force field used in the calculations, for example, CVFF, AMBER force field optimized for proteins, which is contained in DISCOVER module of Insight II program may be used.

Furthermore, the visual examinations and the method by 15 evaluations used in combination energy may be In addition to the visual examination and appropriate. energy examination with computer, complex crystal of the lead compound or compound designed from the lead compound and L-PGDS is analyzed with X-ray crystal analysis. 20 . gives important information for improved evaluation for the fitness between L-PGDA substrate-binding site and compound. Complex crystal is prepared by crystallizing L-PGDS in the solution in which the compound and L-PGDS Alternatively, the crystal of L-PGDS produced in 25 the solution not containing the compound is immersed in the

solution which contains the compound and in which L-PGDS crystal can stably exist. X-ray crystal analysis of the complex crystal can be performed by the method used in the determination of the structure coordinates of native-type Cys⁶⁵Ala L-PGDS. In this case, the analysis can be made using L-PGDS struture coordinates described in Table 2 or 3. If necessary, the method in the determination of the structure coordinates of Se-Met-type L-PGDS may be used.

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After a candidate compound of L-PGDS inhibitor is selected, it is preferably contacted with the enzyme in the presence of the substrate (prostaglandin H_2) to confirm an ability of the compound to inhibit the enzyme (see, for example, Shimizu, t., Yamamoto, S., and Hayaishi O. (1979), Purification and Properties of prostaglandin D synthase from rat brain, J. Biol. Chem., 254:5222-5228). The enzyme activity can be measured, for example, as follows:

[1-14C]prostaglandin The substrate (PG)H₂is reacting [1-14C]arachidonic synthesized by acid cyclooxygenase. Since PGH2 is easily decomposed in an aqueous solution (half life: about 5 minutes), evaporated to dryness and stored at low temperature (-80 $^{\circ}$ C). The enzyme reaction is performed by injecting 1 μ L of PGH₂ solution(acetone or non-volatile diethylenediglycohol solution) with a microsyringe to $49 \mu L$ of 0.1 M phosphate buffer (pH8.0) containing 1 mM dithiothreitol (DTT) and the

enzyme. After the reaction at 25 $^{\circ}$ C for 30 to 60 seconds, the reaction is quenched by the addition of 300 $\mu\,\mathrm{L}$ of icecold mixed solution of ether/methanol/0.1 M citric acid (30:4:1 v/v/v) followed by extraction the substrate and reaction product under acidic condition into ether layer. Subsequently, anhydrous sodium sulfate was added dehydrate it. An aliquot of organic layer (about $50 \mu L$) is coated on silica gel thin layer in a low temperature room $(4^{\circ}C)$ and subjected to silica gel thin layer chromatography (-20 $^{\circ}$) (developing in a freezer solvent: ether/methanol/acetic acid (90:2:1 v/v/v). After the development, radioactivity of PGD2 fraction and fraction other than it are measured to calculate an enzyme activity based on the conversion ratio to PGD2.

After the enzymatic reaction is performed using commercially available non-labeled PGH_2 , PGH_2 is decomposed to 12(S)-hydroxy-8,10-trans-5-cis-heptadecatrienoic acid with $FeCl_2$ treatment followed by reverse phase HPLC using $11-\beta$ — PGE_2 as internal standard to quantify PGD_2 . Commercially available ELISA may be used to quantify PGD_2 .

As described above, the inhibitor can used as pain killer, sleep controlling agent, anti-arteriosclerosis agent, anti-megalocardia agent, antiallergic agent, anti-neurodegenrative agent, and the like

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Examples

Example 1

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Production of L-PGDS

Production of native-type L-PGDS

L-PGDS gene (EMBL/GenBank/DDBJTM Accession No.D83329) from Glu24 to C terminus was obtained from a mouse brain library by PCR amplification and inserted into expression pGEX-2T (Amasham Pharmacia Biotech vector inc.). Escherichia coli DH5 α (Toyobo) was then transformed with the expression vector. pGEX-2T is an expression vector in which a gene of interest is inserted downstream of glutathione (GSH) transferase (GST) gene to express the protein of interest as GST fused protein. In order to prepare Cys65Ala, a pair of synthesized oligomer containing mismatch codon was prepared to replace Cys65 by Ala using the resulting expression vector as a matrix:

5'-GCTGTATTGTATATGgcaAAGACAGTGGTA-3'

5'-TACCACTGTCTTtgcCATATACAATACAGC-3'

In addition, Cys65Ala expression vector was prepared using the Quick change site-directed mutagenesis kit (Stratgene, Heiderberg, Germany). This was bound to glutathione (GSH) transferase (GST) gene (EMBL/GenBank/DDBJ[™] Accession No.U58012) and Escherichia coli DH5 α (Toyobo) was transformed with the expression 25 vector.

L-PGDS prepared by Escherichia coli DH5 α transformed with the expression vector was GST fused protein. transformant is cultured in LB medium at 37° C. When OD600nm reached 0.5-0.6, IPTG is added to 0.6 to 1 mM and L-PGDS was produced at 37° C for 6 hours. Then the transformant was isolated from the medium. The obtained transformant was homogenized by sonication and the resultant supernatant was collected by centrifugation to purify the fused enzyme using GSH-Sepharose 4B column chromatography. The fused enzyme was incubated with thrombin to separate L-PGDS and GST, before subjecting to Superdex 75 column chromatography in 5mM Tris/HCl (pH 8.0) followed by Mono-S chromatography in 10 mM sodium citrate to further purify the enzyme.

The site-specific mutagenesis was performed using a Quick change site-directed mutagenesis kit (Stratgene, Heiderberg, Germany). The DNA sequence was confirmed by the determination of cycle sequencing by a SequiTherm cycle sequencing kit (Epicentre Technologies, Madison, WI) followed by LI-COR model 4000L automatic DNA sequencer (LI-COR Inc., Lincoln, NE)

Production of Se-Met-type L-PGDS

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E. coli B834(DE3) (Novagene, WI, USA) was transformed by PGRX-2T vector obtained as described above, and cultured in the following amino acid-rich medium containing selenomethionine (g/L): alanine 1.5g, arginine HCl 1.75g;

aspartic acid 1.2g; cystein 0.1g; glutamic acid glutamin 1 g; glysine 1.626g; histidine 0.175g; isoleucine 0.7g; leucine 0.7g; lysine HCl 1.26g; phenylalanine 0.4g, proline 0.3g; serine 6.25g, threonine 0.7g; tyrosine 0.5g, valine 0.7g; adenine 1g; guanosine 1.33g; thymine 0.33g; uracyl 1g; sodium acetate 1.5g; succinic acid 3g, ammonium chloride 1.5g, sodium hydroxide 0.85g; K2HPO4 10.5g; Mg SO4 0.25g; FeSO4(II) 0.0042; glucose 20g, selenomethionine 0.075g and Kao Michayluk Basal vitamin solution (Sigma-Aldrich). Before the cultivation in the medium above, the transformant was cultured in 1mL of LB medium at $37^{\circ}C$. mL of the cultured liquid was mixed with 500 mL of the medium above, and further cultured at 37°C overnight. 50 mL of the 500 mL cultured liquid was added to 350 mL of the above fresh medium, and cultured at $37^{\circ}C$. When OD_{600nm} is 0.5-0.6, IPTG was added to 0.6-1 mM and cultivation was continued at 37° C for 12 hours to produce L-PGDS.

Se-Met-type L-PGDS was purified in a similar manner as in native-type L-PGDS.

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Example 2

Crystallization of L-PGDS

The purified enzyme was dialyzed against 5 mM Tris/HCl (pH 8, crystallizing stock solution) and then concentrated to 10 mg/ml through ultra filtration using YM-3 membrane

(Millipore, Badford, MA). Crystallization was effected with hanging drop vapor diffusion method at a constant temperature of 22.5° C.

The native-type $\mathrm{Cys}^{65}\mathrm{Ala}$ L-PGDS was crystallized by mixing 2 μ 1 of the 10 mg/mL enzyme solution with an equal volume of a reservoir solution containing 2 M sodium malonate, 0.1M Tris/HCl (pH8) and 10% (v/v) 1,4-dioxane. Rod form crystal having the maximum size of 0.1 x 0.1 x 0.4 mm was obtained within 3 weeks.

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Se-Met-type L-PGDS Cys⁶⁵Ala L-PGDS was also crystallized by the hanging drop vapor diffusion methods. The liquid drop consisted of 2 μ 1 of the 10 mg/mL enzyme solution containing 10 μ M all-trans retinoic acid and equal volume of mother liquid containing 1.25 M sodium citrate, 10% dioxane, and 2% Triton X-405 in 0.1M Tris/HCl (pH9.5).

Crystallographic parameters were determined using rotating anode-type X-ray generator and Rigaku RAxIS-IV imaging plate system (wave length 1.0000Å)

The native-type L-PGDS has orthorhombic system space group $P2_12_12_1$ and the size of unit cell is a=46.2 Å, b=66.8 Å, and c=105.3 Å. There are two molecules of L-PGDS in crystallographic asymmetrical unit.

The Se-Met-type L-PGDS has orthorhombic system space group C222 $_1$ and the size of unit cell is a=45.7Å, b=66.8Å, and c=104.5 Å . There is one molecule of L-PGDS in

crystallographic asymmetrical unit.

Example 3

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Data Collection and Structure Determination

Diffraction data for Se-Met type and native-type Cys⁶⁵ Ala L-PGDS crystals were collected on Spring-8 Riken beam line I (BL45XU) protein crystallography station at a temperature of 100K. The diffraction data were treated using DENZO and SCALEPACK (Otwinowski et al., Methods Enzymol., 276:307-326 (1997)). CCP4 Sweet (Collaborative Computational Project, Number 4, 1994) was used for successive crystallographic calculation.

Se-Met type Cys⁶⁵Ala L-PGDS crystal belonging to space analyzed with multiwaves C222₁ was anomalous dispersion method. The three sites of selenium were found 15 from difference Patterson map. Phase refinement and electron density modification were carried out using SHARP La Fortelle et al., Methods Enzymol., 276:472-494(1997)) and SOLOMON (Abrahams et al., Acta Crystallogr., 20 D32:32-42 (1996)). Program O (Jones et al., Crystallogr., A47:110-119(1991)) and XtalView (McRee, Practical protein crystallography, Academic Press, 1993) Crystallographic used for model construction. refinement was carried out by the cycle in which refinement calculation in consideration of molecule dynamic using CNS 25

(Brunger et al., Acta Crystallogr., D54:905-921 (1996))) and manual model rectification were alternately effected. Flexible loop region of β barrel portion exhibited weak and unclear electron density. The present model does not include Asn88 of CD loop and 9 N-terminus residues. Crystallographic R and R_{free} for Se-Met enzyme was 0.23 and 0.28 at resolving power of 2.5Å, respectively.

The native-type crystal having P2₁2₁2₁ was solved by followed molecular replacement by crystallographic refinement as above, and then refined by full matrix least squares refinement and manual method. Since CD loop region of one molecule of the two molecules in asymmetrical unit electron density, it was not determined. Crystallographic R and R_{free} for native enzyme was 0.24 and 0.28 at resolving power of 2.1 Å, respectively. The native-type structure of $P2_12_12_1$ has the quite similar structure as Se-Met type protein structure of C2221 except for open EF loop exhibiting deviation of more than 4 Å and Phe³⁹ (whole atoms r.m.s.d=0.26). There are no residues in the region wherein Ramachandran plot of neither structure coordinates are allowed.

The structure coordinates of native-type L-PGDS are shown in Table 2 and those of Se-Met type L-PGDS in Table 3.

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Binding of PGD₂ to L-PGDS

The binding of PGD_2 , PGE_2 or PGF_{2a} to L-PGDS was analyzed with BiaCore 2000 system (BiaCore, Uppsala, Sweden) using the surface plasmon resonance method. L-PGDS mutant Cys^{89,186}Ala was immobilized on CM5 sensor chip (BIAcore AB) coated with carboxymethyldextran. assay was carried out at a constant flow rate of $30 \mu l$ /min. in the concentration range of 0.1 to 10 μ M in both the binding phase and the dissociation phase. After each assay, the sensor chip surface was regenerated with 15 μ l of 1.5 M urea. Rate constant values were calculated using analysis soft wear BIA Evaluation 3.0 soft wear after subtracting control surface (bovine serum albumin) using Langmuir 1: 1 binding model by four independent experiments. The results are shown in Figure 7.

Example 5

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Search of L-PGDS Inhibitor using Three-Dimensional Structure of L-PGDS

Three-dimensional structure of native-type Cys⁶⁵Ala L-PGDS was displayed on a computer screen and three dimensional structures of various compounds were tried to fit to the structure of L-PGDS. As a result, it was found that 4-dibenzo(a,d)cyclohepten-5-ylidene-1-(4-(2H-tetrazole-5-yl)butyl)piperidine (referred to as "AT-56"

hereinafter) having the formula:

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can fit to the three dimensional structure of L-PGDS. AT-56 is in the pocket formed by the amino acid residues of the sites 39, 40, 43, 45, 48, 54, 67, 69, 77, 79, 92, 94, 96, 105, 107, 109, 116, 118, 120, 129, 131, 133, 145, 147, and 149. Among them, the amino acid residues at the sites 45, 92, 147 and 149 is the substrate-binding sites, and therefore AT-56 is a possible inhibitor of L-PGDS.

Inhibition effect of AT-56 on L-PGDS Enzyme Activity

The inhibition effect of AT-56 on L-PGDS enzyme was examined using human recombinant enzyme and the inhibition effect of AT-56 on H-LGDS enzyme was also examined for comparison.

In the measurement of L-PGDS inhibition activity, [1- 14 C]PGH₂ (5 μ M) as substrate is reacted in the presence of human recombinant L-PGDS, 0.1M Tris-HCl (pH 8.0) and 1mM DTT (dithiothreitol) at 25°C for 1 minute.

In the measurement of hematopoietic PGD Synthase (H-PGDS) , [1- 14 C]PGH₂ (40 μ M) as substrate is reacted in the

presence of 0.1 M Tris-HCl (pH 8.0) and 0.1 mM GSH (reduced glutathione) at 25% for 30 seconds.

AT-56 was pretreated for 5 minutes before the addition of the substrate and then the substrate was added. After the completion of the reaction, the reaction liquid was subjected to thin layer chromatography to isolate and quantify PGD₂ to calculate enzyme activity. AT-56 was prepared according to the method described in Japanese Patent Kokai No. 70112/1995, pages 3 and 4.

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The result is shown in Figure 10. AT-56 dose-dependently inhibits the isomerization reaction from PGH₂ to PGD₂ and 50% inhibition concentration (IC₅₀) is 95 μ M. On the other hand, AT-56 (3 to 300 μ M) does not inhibit H-PGDS. It is thus confirmed that At-56 specifically inhibits L-PGDS.

Inhibition Effect of AT-56 on PGD₂ Production from Cell Expressing L-PGDS

The inhibition effect of AT-56 on PGD₂ production by stimulation of calcium ionophore (A23187; 5-(methylamino)- $2[[(2R,3R,6S,8S,9r,11R)-3,9,11-trimethl-8-[(1S)-1-methyl-2-oxo-2-(1H-pyrol-2-yl)ethyl]-1,7-dioxaspiro[5.5]undeca-2-yl]methyl-4-benzoxazole carbonic acid) from human cerebellum medulloblast (TE671) expressing L-PGDS was examined. TE-671 is seeded on microplate at the density of <math>1x10^7$. The cells were stimulated by A231875 (5 μ M) to

cause PGD_2 production. AT-56 or vehicle was added to the cell culture medium 15 minutes before the A23187 stimulation. The culture medium was recovered 15 minutes after A23187 stimulation to quantify the PGD_2 concentration in the culture medium by enzyme immunoassay (EIA).

The results are shown in Figure 11. TE-671 cells increase the production of PGD_2 by the stimulation of A23187 as compared with that without stimulation. The production of PGD2 by A23187 stimulation was dosedependently inhibited by AT-56. The result also confirms that AT-56 is an inhibitor for L-PGDS.

Table 2

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MOTA

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Three Dimensional Coordinates of Native-type L-PGDS

GLN A 35 7.532 25.687 -6.080 1.00 33.40 MOTA 1 N N 15 MOTA CA GLN A 35 7.880 26.161 -4.715 1.00 32.79 C GLN A 35 6.613 26.584 -3.976 1.00 34.50 MOTA CB C GLN A 5.450 25.616 -4.062 1.00 39.74 C MOTA CG 35 -3.369 1.00 49.53 C MOTA 5 $^{\circ}$ GLN A 35 4.209 26.171 OE1 GLN A 35 3.153 25.528 -3.327 1.00 50.48 0 MOTA 20 MOTA NE2 GLN A 35 4.337 27.377 -2.817 1.00 49.93 N MOTA GLN A 8.666 25.154 -3.873 1.00 30.34 C 8 C 35 GLN A 35 9.147 25.489 -2.794 1.00 29.61 0 MOTA 9 0 8.811 23.929 -4.367 MOTA 10 N GLN A 36 1.00 27.61 Ν 36 9.561 22.906 -3.636 1.00 25.74 C CA GLN A MOTA 11

9.751 21.657 -4.503

1.00 24.32

C

CB GLN A 36

	MOTA	13	CG	GLN A	36	10.312	20.473	-3.731	1.00 24.51	С
	ATOM	14	CD	GLN A	36	10.259	19.181	-4.516	1.00 21.94	С
	MOTA	15	OE1	GLN A	36	11.020	18.974	-5.459	1.00 30.10	0
	MOTA	16	NE2	GLN A	36	9.350	18.307	-4.134	1.00 26.53	N
5	MOTA	17	С	GLN A	36	10.930	23.421	-3.170	1.00 23.41	С
	MOTA	18	0	GLN A	36	11.341	23.145	-2.047	1.00 20.27	0
	MOTA	19	N	ASP A	37	11.625	24.162	-4.036	1.00 24.65	N
	MOTA	20	CA	ASP A	37	12.942	24.731	-3.709	1.00 24.97	С
	MOTA	21	СВ	ASP A	37	13.470	25.596	-4.859	1.00 28.96	С
10	MOTA	22	CG	ASP A	37	14.187	24.793	-5.919	1.00 34.20	С
	MOTA	23	OD1	ASP A	37	14.733	25.418	-6.856	1.00 41.87	0
	MOTA	24	OD2	ASP A	37	14.208	23.548	-5.820	1.00 45.04	0
	MOTA	25	С	ASP A	37	12.915	25.597	-2.457	1.00 23.64	С
	MOTA	26	0	ASP A	37	13.938	25.778	-1.795	1.00 23.30	0
15	MOTA	27	N	LYS A	38	11.745	26.137	-2.139	1.00 22.75	N
	MOTA	28	CA	LYS A	38	11.595	26.996	-0.974	1.00 23.00	С
	MOTA	29	СВ	LYS A	38	10.238	27.717	-1.013	1.00 23.35	С
	MOTA	30	CG	LYS A	38	10.024	28.669	-2.185	1.00 23.60	С
	MOTA	31	CD	LYS A	38	10.993	29.825	-2.126	1.00 24.32	С
20	MOTA	32	CE	LYS A	38	10.606	30.923	-3.107	1.00 27.38	С
	MOTA	33	NZ	LYS A	38	9.282	31.485	-2.771	1.00 26.05	N
	MOTA	34	С	LYS A	38	11.704	26.225	0.341	1.00 22.03	С
	MOTA	35	0	LYS A	38	11.980	26.815	1.385	1.00 21.91	0
	ATOM	36	N	PHE A	39	11.501	24.912	0.284	1.00 20.33	N
25	MOTA	37	CA	PHE A	39	11.535	24.079	1.480	1.00 17.56	С

	MOTA	38	СВ	PHE A	39	10.391	23.056	1.442	1.00 19.18	С
	MOTA	39	CG	PHE A	39	9.012	23.676	1.421	1.00 21.95	С
	MOTA	40	CD1	PHE A	39	8.514	24.254	0.263	1.00 16.05	С
	MOTA	41	CE1	PHE A	39	7.233	24.811	0.231	1.00 25.13	С
5	MOTA	42	CZ	PHE A	39	6.442	24.794	1.372	1.00 26.46	С
	MOTA	43	CE2	PHE A	39	6.934	24.219	2.544	1.00 28.59	С
	MOTA	44	CD2	PHE A	39	8.213	23.664	2.561	1.00 25.15	С
	MOTA	45	С	PHE A	39	12.860	23.359	1.692	1.00 18.10	С
	MOTA	46	0	PHE A	39	12.999	22.536	2.598	1.00 15.86	0
10	MOTA	47	N	LEU A	40	13.840	23.662	0.855	1.00 17.02	N
	MOTA	48	CA	LEU A	40	15.140	23.037	1.001	1.00 17.96	С
	MOTA	49	СВ	LEU A	40	16.034	23.360	-0.198	1.00 17.02	С
	MOTA	50	CG	LEU A	40	15.501	22.886	-1.546	1.00 20.11	С
	MOTA	51	CD1	LEU A	40	16.493	23.229	-2.659	1.00 20.64	С
15	MOTA	52	CD2	LEU A	40	15.266	21.391	-1.481	1.00 15.79	С
	MOTA	53	, C	LEU A	40	15.750	23.602	2.271	1.00 17.56	С
	MOTA	54	0	LEU A	40	15.202	24.528	2.874	1.00 17.30	0
	ATOM	55	N	GLY A	41	16.861	23.019	2.702	1.00 16.10	N
	ATOM	56	CA	GLY A	41	17.521	23.531	3.888	1.00 15.92	Ċ
20	MOTA	57	С	GLY A	41	17.293	22.823	5.207	1.00 15.14	С
	ATOM	58	0	GLY A	41	16.873	21.667	5.253	1.00 17.51	0
	ATOM	59	N	ARG A	42	17.564	23.550	6.289	1.00 15.43	N
	ATOM	60	CA	ARG A	42	17.461	23.028	7.645	1.00 17.08	С
	ATOM	61	СВ	ARG A	42	18.509	23.721	8.538	1.00 15.38	С
25	MOTA	62	CG	ARG A	42	18.574	23.214	9.995	1.00 15.81	С

	MOTA	63	CD	ARG A	42	19.475	24.086	10.917	1.00 17.38	С
	MOTA	64	NE	ARG A	42	18.931	25.430	11.127	1.00 20.69	N
	MOTA	65	CZ	ARG A	42	19.516	26.393	11.846	1.00 24.91	С
	MOTA	66	NH1	ARG A	42	20.676	26.180	12.449	1.00 18.52	N
5	MOTA	67	NH2	ARG A	42	18.946	27.591	11.948	1.00 23.29	N
	MOTA	68	С	ARG A	42	16.093	23.133	8.320	1.00 16.71	С
	MOTA	69	0	ARG A	42	15.490	24.209	8.393	1.00 17.77	0
	MOTA	70	N	TRP A	43	15.627	22.001	8.836	1.00 17.28	N
	MOTA	71	CA	TRP A	43	14.356	21.939	9.552	1.00 18.13	С
10	MOTA	72	СВ	TRP A	43	13.283	21.239	8.721	1.00 15.45	С
	MOTA	73	CG	TRP A	43	12.856	21.946	7.485	1.00 15.71	С
	ATOM	74	CD1	TRP A	43	13.401	21.834	6.233	1.00 15.15	С
	MOTA	75	NE1	TRP A	43	12.662	22.576	5.330	1.00 15.14	N
	MOTA	76	CE2	TRP A	43	11.631	23.187	5.996	1.00 14.06	С
15	MOTA	77	CD2	TRP A	43	11.721	22.817	7.357	1.00 12.61	С
	MOTA	78	CE3	TRP A	43	10.778	23.319	8.264	1.00 14.15	С
	MOTA	79	CZ3	TRP A	43	9.777	24.162	7.792	1.00 11.66	С
	MOTA	80	CH2	TRP A	43	9.709	24.512	6.426	1.00 15.44	С
	MOTA	81	CZ2	TRP A	43	10.626	24.034	5.520	1.00 15.17	С
20	MOTA	82	С	TRP A	43	14.565	21.126	10.821	1.00 18.08	С
	MOTA	83 .	0	TRP A	43	15.587	20.460	10.981	1.00 18.87	0
	ATOM	84	N	TYR A	44	13.583	21.173	11.710	1.00 19.02	N
	MOTA	85	CA	TYR A	44	13.617	20.413	12.952	1.00 19.64	С
	ATOM	86	СВ	TYR A	44	13.822	21.335	14.154	1.00 19.30	С
25	ATOM	87	CG	TYR A	44	15.113	22.102	14.146	1.00 20.96	С

	MOTA	88	CD1	TYR A	44	16.306	21.494	14.524	1.00 21.90	С
	ATOM	89	CE1	TYR A	44	17.506	22.194	14.501	1.00 26.37	С
	MOTA	90	CZ	TYR A	44	17.512	23.521	14.094	1.00 28.61	С
	MOTA	91	ОН	TYR A	44	18.690	24.228	14.082	1.00 31.66	0
5	MOTA	92	CE2	TYR A	44	16.338	24.145	13.710	1.00 26.67	С
	MOTA	93	CD2	TYR A	44	15.146	23.434	13.740	1.00 21.12	С
	MOTA	94	С	TYR A	44	12.270	19.717	13.120	1.00 18.71	С
	ATOM	95	0	TYR A	44	11.221	20.356	12.993	1.00 18.76	0
	ATOM	96	N	SER A	45	12.300	18.413	13.388	1.00 20.71	N
10	MOTA	97	CA	SER A	45	11.072	17.658	13.625	1.00 20.41	С
	MOTA	98	СВ	SER A	45	11.349	16.153	13.541	1.00 21.74	С
	MOTA	99	œ	SER A	45	12.516	15.802	14.276	1.00 19.43	0
	MOTA	100	С	SER A	45	10.671	18.051	15.045	1.00 21.87	С
	MOTA	101	0	SER A	45	11.377	17.735	16.005	1.00 23.08	0
15	ATOM	102	N	ALA A	46	9.553	18.764	15.171	1.00 21.80	N
	ATOM	103	CA	ALA A	46	9.073	19.239	16.464	1.00 20.98	С
	MOTA	104	СВ	ALA A	46	8.868	20.756	16.402	1.00 20.73	С
	MOTA	105	С	ALA A	46	7.791	18.570	16.945	1.00 21.49	С
	ATOM	106	0	ALA A	46	7.464	18.635	18.127	1.00 22.81	0
20	ATOM	107	N	GLY A	47	7.053	17.947	16.034	1.00 21.44	N
	ATOM	108	CA	GLY A	47	5.811	17.293	16.420	1.00 21.24	С
	MOTA	109	С	GLY A	47	5.614	15.989	15.682	1.00 20.50	С
	ATOM	110	0	GLY A	47	5.926	15.895	14.495	1.00 21.41	0
	ATOM	111	N	LEU A	48	5.106	14.976	16.376	1.00 22.43	N
25	ATOM	112	CA	LEU A	48	4.879	13.674	15.755	1.00 24.18	С

	MOTA	113	СВ	LEU A	48	6.119	12.796	15.952	1.00 24.03	С
	ATOM	114	CG	LEU A	48	6.216	11.439	15.258	1.00 25.64	С
	ATOM	115	CD1	LEU A	48	6.256	11.620	13.745	1.00 23.98	С
	MOTA	116	CD2	LEU A	48	7.490	10.732	15.731	1.00 24.77	С
5	MOTA	117	С	LEU A	48	3.646	12.997	16.353	1.00 25.73	С
	MOTA	118	0	LEU A	48	3.460	12.988	17.568	1.00 28.24	0
	ATOM	119	N	ALA A	49	2.800	12.438	15.492	1.00 26.62	N
	MOTA	120	CA	ALA A	49	1.590	11.755	15.934	1.00 27.70	С
	ATOM	121	СВ	ALA A	49	0.408	12.706	15.893	1.00 26.11	С
10	ATOM	122	С	ALA A	49	1.337	10.556	15.029	1.00 29.92	С
	ATOM	123	0	ALA A	49	1.610	10.612	13.829	1.00 30.06	0
	ATOM	124	N	SER A	50	0.825	9.470	15.604	1.00 33.10	N
	MOTA	125	CA	SER A	50	0.556	8.266	14.823	1.00 35.56	С
	ATOM	126	СВ	SER A	50	1.874	7.657	14.346	1.00 34.98	C .
15	MOTA	127	Œ	SER A	50	1.648	6.580	13.458	1.00 37.15	0
	ATOM	128	С	SER A	50	-0.233	7.214	15.600	1.00 37.86	С
	MOTA	129	0	SER A	50	-0.427	7.333	16.813	1.00 39.05	0
	MOTA	130	N	ASN A	51	-0.693	6.185	14.888	1.00 39.58	N
	MOTA	131	CA	ASN A	51	-1.447	5.091	15.509	1.00 41.56	С
20	MOTA	132	СВ	ASN A	51	-2.817	4.940	14.841	1.00 41.04	С
	MOTA	133	CG	ASN A	51	-2.718	4.653	13.354	1.00 42.05	С
	MOTA	134	OD1	asn a	51	-3.726	4.392	12.698	1.00 45.32	0
	MOTA	135	ND2	ASN A	51	-1.511	4.706	12.816	1.00 39.99	N
	ATOM	136	С	ASN A	51	-0.658	3.790	15.361	1.00 43.28	С
25	MOTA	137	0	ASN A	51	-1.097	2.723	15.788	1.00 43.84	0

	MOTA	138	N	SER A	52	0.516	3.901	14.751	1.00 45.47	N
	MOTA	139	CA	SER A	52	1.387	2.760	14.514	1.00 47.77	С
	MOTA	140	СВ	SER A	52	2.663	3.228	13.815	1.00 48.05	,C
	MOTA	141	Œ	SER A	52	3.599	2.173	13.701	1.00 51.48	0
5	MOTA	142	С	SER A	52	1.755	2.027	15.796	1.00 48.61	С
	MOTA	143	0	SER A	52	1.395	2.444	16.895	1.00 49.34	0
	MOTA	144	N	SER A	53	2.475	0.923	15.636	1.00 49.72	N
	MOTA	145	CA	SER A	53	2.933	0.118	16.762	1.00 50.37	С
	MOTA	146	СВ	SER A	53	3.129	-1.340	16.333	1.00 50.55	С
10	MOTA	147	Œ	SER A	53	1.912	-1.919	15.891	1.00 52.17	0
	MOTA	148	С	SER A	53	4.270	0.704	17.190	1.00 50.30	С
	MOTA	149	0	SER A	53	4.579	0.805	18.379	1.00 50.13	0
	ATOM	150	N	TRP A	54	5.056	1.082	16.188	1.00 50.56	N
	MOTA	151	CA	TRP A	54	6.372	1.678	16.380	1.00 50.79	С
15	MOTA	152	СВ	TRP A	54	6.930	2.116	15.022	1.00 51.39	С
	MOTA	153	CG	TRP A	54	8.264	2.783	15.090	1.00 - 54.05	С
	MOTA	154	CD1	TRP A	54	9.472	2.183	15.300	1.00 55.89	С
	MOTA	155	NE1	TRP A	54	10.473	3.124	15.315	1.00 56.28	N
	MOTA	156	CE2	TRP A	54	9.922	4.362	15.114	1.00 57.18	С
20	MOTA	157	CD2	TRP A	54	8.529	4.186	14.966	1.00 56.11	С
	MOTA	158	CE3	TRP A	54	7.724	5.313	14.746	1.00 57.68	С
	MOTA	159	CZ3	TRP A	54	8.330	6.564	14.681	1.00 56.58	С
	MOTA	160	CH2	TRP A	54	9.721	6.706	14.833	1.00 57.14	С
	MOTA	161	CZ2	TRP A	54	10.531	5.621	15.049	1.00 57.71	С
25	MOTA	162	С	TRP A	54	6.261	2.889	17.301	1.00 49.63	С

	ATOM	163	0	TRP A	54	6.870	2.935	18.374	1.00 48.99	0
	MOTA	164	N	PHE A	55	5.470	3.865	16.868	1.00 48.67	N
	MOTA	165	CA	PHE A	55	5.268	5.091	17.625	1.00 47.55	С
	MOTA	166	СВ	PHE A	55	4.228	5.972	16.928	1.00 47.41	С
5	MOTA	167	CG	PHE A	55	4.014	7.298	17.599	1.00 46.06	С
	MOTA	168	CD1	PHE A	55	5.020	8.258	17.606	1.00 47.31	С
	MOTA	169	CE1	PHE A	55	4.833	9.479	18.241	1.00 45.75	С
	ATOM	170	CZ	PHE A	55	3.633	9.750	18.875	1.00 45.84	С
	MOTA	171	CE2	PHE A	55	2.621	8.798	18.874	1.00 44.73	С
10	ATOM	172	CD2	PHE A	55	2.816	7.582	18.238	1.00 44.94	С
	ATOM	173	С	PHE A	55	4.822	4.805	19.054	1.00 47.07	С
	ATOM	174	0	PHE A	55	5.415	5.305	20.011	1.00 45.46	0
	ATOM	175	N	ARG A	56	3.775	3.997	19.193	1.00 47.71	N
	MOTA	176	CA	ARG A	56	3.243	3.654	20.509	1.00 48.60	С
15	MOTA	177	СВ	ARG A	56	2.030	2.732	20.354	1.00 49.22	С
	MOTA	178	CG	ARG A	56	0.822	3.456	19.777	1.00 51.68	С
	MOTA	179	CD	ARG A	56	-0.320	2.516	19.428	1.00 56.98	С
	MOTA	180	NE	ARG A	56	-1.471	3.257	18.913	1.00 59.80	N
	ATOM	181	CZ	ARG A	56	-2.578	2.693	18.444	1.00 61.91	С
20	ATOM	182	NH1	ARG A	56	-2.691	1.373	18.421	1.00 62.67	N
	ATOM	183	NH2	ARG A	56	-3.575	3.449	18.000	1.00 62.84	N
	MOTA	184	С	ARG A	56	4.279	3.019	21.426	1.00 48.38	С
	MOTA	185	0	ARG A	56	4.270	3.256	22.634	1.00 48.01	0
	MOTA	186	N	GLU A	57	5.183	2.230	20.854	1.00 47.94	N
25	MOTA	187	CA	GLU A	57	6.209	1.573	21.652	1.00 48.73	С

	MOTA	188	СВ	GLU A	57	6.275	0.082	21.306	1.00 49.15	С
	MOTA	189	CG	GLU A	57	4.958	-0.663	21.500	1.00 50.89	С
	MOTA	190	CD	GLU A	57	5.110	-2.170	21.373	1.00 53.24	С
	MOTA	191	OE1	GLU A	57	5.686	-2.632	20.363	1.00 53.06	0
5	MOTA	192	OE2	GLU A	57	4.649	-2.893	22.285	1.00 56.31	0
	MOTA	193	С	GLU A	57	7.602	2.188	21.514	1.00 48.51	С
	MOTA	194	0	GLU A	57	8.602	1.489	21.668	1.00 48.84	0
	MOTA	195	N	LYS A	58	7.668	3.487	21.234	1.00 47.64	N
	MOTA	196	CA	LYS A	58	8.950	4.177	21.096	1.00 46.97	С
10	MOTA	197	CB	LYS A	58	9.579	3.882	19.729	1.00 48.03	С
	MOTA	198	CG	LYS A	58	10.147	2.475	19.597	1.00 51.08	С
	MOTA	199	CD	LYS A	58	10.780	2.245	18.239	1.00 56.50	С
	MOTA	200	CE	LYS A	58	11.185	0.787	18.060	1.00 58.17	С
	MOTA	201	NZ	LYS A	58	11.672	0.506	16.677	1.00 59.90	N
15	MOTA	202	С	LYS A	58	8.826	5.683	21.277	1.00 45.19	С
	MOTA	203	O	LYS A	58	9.833	6.388	21.334	1.00 44.57	0
	ATOM	204	N	LYS A	59	7.592	6.169	21.371	1.00 43.70	N
	MOTA	205	CA ·	LYS A	59	7.326	7.596	21.532	1.00 42.75	С
	ATOM	206 -	CB	LYS A	59	5.827	7.826	21.698	1.00 43.46	С
20	MOTA	207	CG	LYS A	59	5.236	7.188	22.944	1.00 45.39	С
	ATOM	208	CD	LYS A	59	3.713	7.187	22.902	1.00 48.36	С
	ATOM	209	CE	LYS A	59	3.153	8.591	22.714	1.00 50.84	С
	ATOM	210	NZ	LYS A	59	3.580	9.517	23.798	1.00 50.65	N
	MOTA	211	С	LYS A	59	8.069	8.211	22.714	1.00 41.89	С
25	ATOM	212	0	LYS A	59	8.541	9.345	22.641	1.00 41.05	0

	ATOM	213	N	ALA A	60	8.176	7.457	23.802	1.00 40.68	N
	ATOM	214	CA	ALA A	60	8.858	7.936	24.996	1.00 39.93	С
	ATOM	215	СВ	ALA A	60	8.704	6.923	26.124	1.00 39.51	С
	ATOM	216	С	ALA A	60	10.338	8.235	24.768	1.00 39.23	С
5	ATOM	217	0	ALA A	60	10.897	9.104	25.436	1.00 39.44	0
	ATOM	218	N	VAL A	61	10.970	7.525	23.833	1.00 37.14	N
	ATOM	219	CA	VAL A	61	12.395	7.726	23.560	1.00 35.90	С
	MOTA	220	СВ	VAL A	61	13.141	6.380	23.339	1.00 36.11	С
	ATOM	221	CG1	VAL A	61	12.952	5.463	24.537	1.00 34.24	С
10	ATOM	222	CG2	VAL A	61	12.655	5.721	22.063	1.00 35.38	С
	ATOM	223	С	VAL A	61	12.698	8.602	22.351	1.00 35.45	С
	MOTA	224	0	VAL A	61	13.856	8.716	21.940	1.00 35.12	0
	MOTA	225	N	LEU A	62	11.670	9.219	21.778	1.00 33.84	N
	ATOM	226	CA	LEU A	62	11.873	10.074	20.614	1.00 32.75	С
15	MOTA	227	СВ	LEU A	62	10.621	10.062	19.734	1.00 33.05	С
	ATOM	228	CG	LEU A	62	10.265	8.671	19.212	1.00 35.96	С
	ATOM	229	CD1	LEU A	62	9.046	8.756	18.313	1.00 34.96	С
	ATOM	230	CD2	LEU A	62	11.457	8.086	18.460	1.00 39.51	С
	ATOM	231	С	LEU A	62	12.242	11.512	20.970	1.00 30.66	С
20	ATOM	232	0	LEU A	62	11.663	12.113	21.872	1.00 30.48	0
	ATOM	233	N	TYR A	63	13.226	12.053	20.261	1.00 29.47	N
	ATOM	234	CA	TYR A	63	13.658	13.425	20.484	1.00 27.67	С
	ATOM	235	СВ	TYR A	63	15.103	13.481	21.003	1.00 29.10	С
	ATOM	236	CG	TYR A	63	15.316	12.881	22.378	1.00 31.25	С
25	ATOM	237	CD1	TYR A	63	15.441	11.503	22.549	1.00 33.47	С

	ATOM	238	CE1	TYR A	63	15.642	10.948	23.810	1.00 39.12	С
	ATOM	239	CZ	TYR A	63	15.716	11.776	24.922	1.00 38.97	С
	ATOM	240	OH	TYR A	63	15.905	11.223	26.175	1.00 44.99	0
	ATOM	241	CE2	TYR A	63	15.593	13.152	24.776	1.00 37.23	С
5	ATOM	242	CD2	TYR A	63	15.394	13.694	23.508	1.00 32.70	С
	MOTA	243	С	TYR A	63	13.582	14.202	19.181	1.00 25.92	С
	ATOM	244	0	TYR A	63	13.420	13.628	18.107	1.00 26.31	0
	MOTA	245	N	MET A	64	13.705	15.517	19.289	1.00 24.98	N
	ATOM	246	CA	MET A	64	13.685	16.381	18.127	1.00 22.50	C
10	ATOM	247	СВ	MET A	64	13.755	17.838	18.549	1.00 21.53	С
	ATOM	248	CG	MET A	64	14.062	18.792	17.408	1.00 23.46	С
	ATOM	249	SD	MET A	64	14.026	20.469	17.999	1.00 24.75	S
	ATOM	250	CE	MET A	64	12.269	20.682	18.254	1.00 26.17	С
	ATOM	251	С	MET A	64	14.898	16.059	17.299	1.00 21.60	С
15	ATOM	252	0	MET A	64	15.984	15.876	17.840	1.00 20.32	0
	ATOM	253	N	ALA A	65	14.714	16.000	15.984	1.00 21.77	N
	ATOM	254	CA	ALA A	65	15.801	15.702	15.071	1.00 21.68	С
	ATOM	255	СВ	ALA A	65	15.484	14.450	14.268	1.00 22.60	С
	ATOM	256	С	ALA A	65	16.048	16.866	14.130	1.00 21.03	С
20	MOTA	257	0	ALA A	65	15.154	17.670	13.870	1.00 20.19	0
	MOTA	258	N	LYS A	66	17.274	16.959	13.633	1.00 22.99	N
	ATOM	259	CA	LYS A	66	17.626	18.010	12.693	1.00 22.22	С
	MOTA	260	СВ	LYS A	66	19.024	18.564	12.967	1.00 23.06	С
	ATOM	261	CG	LYS A	66	19.499	19.477	11.847	1.00 24.65	С
25	MOTA	262	CD	LYS A	66	21.009	19.641	11.800	1.00 30.24	С

	MOTA	263	CE	LYS A	66	21.462	20.820	12.622	1.00 35.63	С
	MOTA	264	NZ	LYS A	66	22.848	21.237	12.231	1.00 43.47	N
	MOTA	265	С	LYS A	66	17.608	17.356	11.326	1.00 23.44	С
	MOTA	266	0	LYS A	66	18.312	16.375	11.091	1.00 24.56	0
5	MOTA	267	N	THR A	67	16.802	17.898	10.427	1.00 20.70	N
	MOTA	268	CA	THR A	67	16.690	17.344	9.085	1.00 20.77	C
	MOTA	269	СВ	THR A	67	15.235	16.874	8.816	1.00 19.10	С
	MOTA	270	OG1	THR A	67	14.823	16.005	9.868	1.00 22.20	0
	MOTA	271	CG2	THR A	67	15.137	16.133	7.516	1.00 22.53	С
10	MOTA	272	С	THR A	67	17.085	18.378	8.030	1.00 19.13	С
	MOTA	273	0	THR A	67	16.536	19.483	7.992	1.00 19.67	0
	MOTA	274	N	VAL A	68	18.047	18.016	7.189	1.00 17.58	N
	MOTA	275	CA	VAL A	68	18.494	18.900	6.120	1.00 18.47	С
	MOTA	276	СВ	VAL A	68	20.042	18.944	6.026	1.00 16.97	С
15	MOTA	277	CG1	VAL A	68	20.480	19.900	4.914	1.00 19.31	С
	MOTA	278	CG2	VAL A	68	20.622	19.408	7.349	1.00 17.36	С
	MOTA	279	С	VAL A	68	17.891	18.378	4.824	1.00 16.74	С
	MOTA	280	0	VAL A	68	18.012	17.198	4.496	1.00 17.78	0
	MOTA	281	N	VAL A	69	17.235	19.271	4.095	1.00 15.74	N
20	MOTA	282	CA	VAL A	69	16.565	18.904	2.860	1.00 14.97	С
	MOTA	283	СВ	VAL A	69	15.113	19.412	2.894	1.00 16.13	С
	MOTA	284	CG1	VAL A	69	14.370	18.984	1.643	1.00 18.02	С
	ATOM	285	CG2	VAL A	69	14.417	18.867	4.145	1.00 15.17	С
	ATOM	286	С	VAL A	69	17.250	19.405	1.595	1.00 14.61	С
25	ATOM	287	0	VAL A	69	17.645	20.560	1.504	1.00 14.02	0

	MOTA	288	N	ALA A	70	17.387	18.519	0.616	1.00 15.92	N
	MOTA	289	CA	ALA A	70	18.015	18.856	-0.661	1.00 16.00	С
	MOTA	290	СВ	ALA A	70	19.513	18.524	-0.618	1.00 17.37	С
	MOTA	291	С	ALA A	70	17.316	18.054	-1.749	1.00 15.57	С
5	MOTA	292	0	ALA A	70	16.585	17.110	-1.452	1.00 17.54	0
	MOTA	293	N	PRO A	71	17.535	18.411	-3.023	1.00 15.95	N
	MOTA	294	CA	PRO A	71	16.886	17.686	-4.123	1.00 16.43	С
	MOTA	295	СВ	PRO A	71	17.345	18.453	-5.369	1.00 16.22	С
	MOTA	296	CG	PRO A	71	17.689	19.839	-4.838	1.00 17.77	С
10	MOTA	297	CD	PRO A	71	18.362	19.521	-3.536	1.00 15.68	С
	MOTA	298	С	PRO A	71	17.257	16.216	-4.204	1.00 16.59	С
	ATOM	299	0	PRO A	71	18.367	15.841	-3.853	1.00 16.86	0
	MOTA	300	N	SER A	72	16.320	15.391	-4.665	1.00 18.06	N
	MOTA	301	CA	SER A	72	16.567	13.972	-4.830	1.00 18.01	С
15	MOTA	302	СВ	SER A	72	15.367	13.145	-4.367	1.00 19.58	С
	ATOM	303	OG	SER A	72	14.336	13.166	-5.335	1.00 21.44	0
	ATOM .	304	С	SER A	72	16.805	13.759	-6.322	1.00 18.75	С
	MOTA	305	0	SER A	72	16.501	14.637	-7.133	1.00 16.43	0
	ATOM	306	N	THR A	73	17.347	12.597	-6.679	1.00 18.47	N
20	ATOM	307	CA	THR A	73	17.654	12.272	-8.075	1.00 20.83	С
	ATOM	308	СВ	THR A	73	18.125	10.806	-8.218	1.00 20.62	С
	ATOM	309	OG1	THR A	73	19.179	10.534	-7.285	1.00 16.43	0
	MOTA	310	CG2	THR A	73	18.617	10.550	-9.632	1.00 22.06	С
	ATOM	311	С	THR A	73	16.495	12.451	-9.053	1.00 24.09	С
25	MOTA	312	0	THR A	73	16.659	13.062	-10.117	1.00 25.21	0

	MOTA	313	N	GLU A	74	15.334	11.908	-8.687	1.00 25.04	N
	ATOM	314	CA	GLU A	74	14.138	11.929	-9.533	1.00 25.92	С
	ATOM	315	СВ	GLU A	74	13.236	10.750	-9.159	1.00 26.06	С
	MOTA	316	CG	GLU A	74	12.406	10.178	-10.286	1.00 34.32	С
5	MOTA	317	CD	GLU A	74	13.256	9.541	-11.370	1.00 38.16	С
	ATOM	318	OE1	GLU A	74	14.199	8.801	-11.024	1.00 41.27	0
	MOTA	319	OE2	GLU A	74	12.975	9.771	-12.568	1.00 40.53	0
	MOTA	320	С	GLU A	74	13.333	13.217	-9.440	1.00 26.08	С
	MOTA	321	0	GLU A	74	12.262	13.321	-10.025	1.00 24.26	0
10	MOTA	322	N	GLY A	75	13.840	14.194	-8.701	1.00 26.42	N
	MOTA	323	CA	GLY A	75	13.117	15.445	-8.570	1.00 22.94	С
	MOTA	324	С	GLY A	75	12.382	15.554	-7.247	1.00 23.36	С
	MOTA	325	0	GLY A	75	11.727	16.566	-6.979	1.00 23.95	0
	MOTA	326	N	GLY A	76	12.478	14.509	-6.427	1.00 21.05	N
15	MOTA	327	CA	GLY A	76	11.831	14.516	-5.123	1.00 19.01	С
	MOTA	328	С	GLY A	76	12.760	15.147	-4.095	1.00 18.58	С
	MOTA	329	0	GLY A	76	13.564	16.004	-4.450	1.00 18.03	0
	MOTA	330	N	LEU A	77	12.672	14.723	-2.834	1.00 17.32	N
	ATOM	331	CA	LEU A	77	13.518	15.288	-1.789	1.00 16.39	С
20	ATOM	332	СВ	LEU A	77	12.663	16.094	-0.804	1.00 17.26	С
	MOTA	333	CG	LEU A	77	11.836	17.252	-1.368	1.00 18.75	С
	ATOM	334	CD1	LEU A	77	10.833	17.685	-0.329	1.00 21.30	С
	ATOM	335	CD2	LEU A	77	12.741	18.423	-1.794	1.00 17.34	С
	ATOM	336	С	LEU A	77	14.354	14.293	-0.987	1.00 17.25	С
25	ATOM	337	0	LEU A	77	13.886	13.223	-0.602	1.00 17.86	0

	MOTA	338	N	ASN A	78	15.603	14.676	-0.741	1.00 16.40	N
	MOTA	339	CA	ASN A	78	16.521	13.884	0.062	1.00 16.85	С
	MOTA	340	СВ	ASN A	78	17.966	14.049	-0.421	1.00 17.82	С
	MOTA	341	CG	ASN A	78	18.362	13.029	-1.456	1.00 16.18	С
5	MOTA	342	OD1	ASN A	78	17.533	12.293	-1.972	1.00 14.36	0
	MOTA	343	ND2	ASN A	78	19.653	12.982	-1.767	1.00 16.85	N
	MOTA	344	С	ASN A	78	16.401	14.508	1.444	1.00 18.05	С
	MOTA	345	0	ASN A	78	16.472	15.730	1.573	1.00 17.02	0
	MOTA	346	N	LEU A	79	16.202	13.682	2.463	1.00 17.20	N
10	MOTA	347	CA	LEU A	79	16.096	14.161	3.829	1.00 17.68	С
	MOTA	348	СВ	LEU A	79	14.717	13.826	4.427	1.00 19.58	С
	MOTA	349	CG	LEU A	79	13.572	14.852	4.291	1.00 19.99	С
	MOTA	350	CD1	LEU A	79	13.158	15.002	2.851	1.00 17.35	С
	MOTA	351	CD2	LEU A	79	12.386	14.413	5.126	1.00 21.80	С
15	MOTA	352	С	LEU A	79	17.196	13.480	4.642	1.00 18.93	С
	MOTA	353	0	LEU A	79	17.177	12.264	4.833	1.00 17.64	0
	MOTA	354	N	THR A	80	18.167	14.271	5.096	1.00 18.20	N
	MOTA	355	CA	THR A	80	19.265	13.749	5.896	1.00 18.43	С
	ATOM	356	СВ	THR A	80	20.616	14.317	5.406	1.00 17.16	С
20	ATOM	357	OG1	THR A	80	20.805	13.949	4.029	1.00 17.30	0
	MOTA	358	CG2	THR A	80	21.772	13.765	6.241	1.00 17.81	С
	ATOM	359	С	THR A	80	18.987	14.174	7.327	1.00 19.48	С
	MOTA	360	0	THR A	80	19.005	15.360	7.649	1.00 19.03	0
	ATOM	361	N	SER A	81	18.698	13.201	8.181	1.00 19.91	N
25	ATOM	362	CA	SER A	81	18.383	13.489	9.569	1.00 22.53	С

	MOTA	363	СВ	SER A	81	17.027	12.867	9.945	1.00 23.42	С
	MOTA	364	œ	SER A	81	15.958	13.406	9.166	1.00 25.72	0
	MOTA	365	С	SER A	81	19.443	13.015	10.554	1.00 24.28	С
	MOTA	366	0	SER A	81	20.011	11.920	10.425	1.00 25.45	0
5	MOTA	367	N	THR A	82	19.703	13.870	11.532	1.00 25.36	N
	MOTA	368	CA	THR A	82	20.655	13.602	12.596	1.00 27.24	С
	MOTA	369	СВ	THR A	82	21.618	14.791	12.787	1.00 26.98	С
	MOTA	370	OG1	THR A	82	22.329	15.034	11.566	1.00 30.38	0
	MOTA	371	CG2	THR A	82	22.616	14.501	13.905	1.00 27.31	С
10	MOTA	372	С	THR A	82	19.779	13.460	13.840	1.00 28.34	С
	MOTA	373	Ο.	THR A	82	19.031	14.381	14.176	1.00 28.53	0
	MOTA	374	N	PHE A	83	19.866	12.317	14.519	1.00 29.40	N
	MOTA	375	CA	PHE A	83	19.043	12.076	15.700	1.00 31.45	С
	MOTA	376	СВ	PHE A	83	17.748	11.382	15.279	1.00 32.44	С
15	MOTA	377	CG	PHE A	83	17.968	10.118	14.493	1.00 33.67	С
	MOTA	378	CD1	PHE A	83	18.310	10.171	13.146	1.00 32.21	С
	MOTA	379	CE1	PHE A	83	18.532	9.005	12.418	1.00 35.94	С
	MOTA	380	CZ	PHE A	83	18.415	7.766	13.037	1.00 35.35	С
	MOTA	381	CE2	PHE A	83	18.075	7.699	14.382	1.00 37.16	С
20	MOTA	382	CD2	PHE A	83	17.853	8.873	15.104	1.00 33.77	С
	MOTA	383	С	PHE A	83	19.715	11.249	16.797	1.00 33.26	С
	MOTA	384	0	PHE A	83	20.721	10.571	16.569	1.00 33.27	0
	MOTA	385	N	LEU A	84	19.137	11.315	17.991	1.00 35.25	N
	MOTA	386	CA	LEU A	84	19.633	10.578	19.148	1.00 37.42	С
25	MOTA	387	СВ	LEU A	84	19.424	11.413	20.415	1.00 37.09	С

	MOTA	388	CG	LEU A	84	19.882	10.858	21.769	1.00 39.37	С
	MOTA	389	CD1	LEU A	84	21.401	10.658	21.774	1.00 37.77	С
	MOTA	390	CD2	LEU A	84	19.467	11.824	22.870	1.00 39.73	С
	MOTA	391	С	LEU A	84	18.836	9.272	19.226	1.00 39.36	С
5	MOTA	392	0	LEU A	84	17.620	9.292	19.415	1.00 38.00	0
	MOTA	393	N	ARG A	85	19.524	8.145	19.062	1.00 42.28	N
	MOTA	394	CA	ARG A	85	18.887	6.828	19.092	1.00 46.17	С
	MOTA	395	СВ	ARG A	85	19.617	5.895	18.124	1.00 47.06	С
	MOTA	396	CG	ARG A	85	19.280	4.412	18.240	1.00 50.03	С
10	MOTA	397	CD	ARG A	85	17.975	4.035	17.555	1.00 54.72	С
	MOTA	398	NE	ARG A	85	18.016	2.648	17.088	1.00 59.25	N
	MOTA	399	CZ	ARG A	85	16.987	1.994	16.553	1.00 60.78	С
	MOTA	400	NH1	ARG A	85	15.812	2.596	16.410	1.00 62.71	N
	MOTA	401	NH2	ARG A	85	17.135	0.736	16.154	1.00 59.48	N
15	MOTA	402	С	ARG A	85	18.894	6.224	20.493	1.00 48.27	С
	MOTA	403	Ο.	ARG A	85	17.842	5.982	21.096	1.00 49.91	Ο.
	MOTA	404	N	LYS A	86	20.094	5.966	20.999	1.00 49.22	N
	MOTA	405	CA	LYS A	86	20.266	5.397	22.329	1.00 50.08	С
	MOTA	406	СВ	LYS A	86	20.385	3.873	22.242	1.00 50.26	С
20	MOTA	407	CG	LYS A	86	19.188	3.195	21.587	1.00 52.36	С
	MOTA	408	CD	LYS A	86	19.420	1.702	21.391	1.00 54.20	С
	MOTA	409	CE	LYS A	86	18.224	1.049	20.709	1.00 56.17	С
	MOTA	410	NZ	LYS A	86	18.420	-0.410	20.487	1.00 57.21	N
	ATOM	411	С	LYS A	86	21.550	5.991	22.882	1.00 50.00	С
25	ATOM	412	0	LYS A	86	22.583	5.323	22.939	1.00 49.77	0

	MOTA	413	N	ASN A	87	21.478	7.260	23.273	1.00 50.54	N
	MOTA	414	CA	ASN A	87	22.632	7.974	23.800	1.00 50.72	С
	ATOM	415	СВ	ASN A	87	23.159	7.284	25.063	1.00 51.47	С
	MOTA	416	CG	ASN A	87	22.168	7.337	26.219	1.00 52.54	С
5	MOTA	417	OD1	ASN A	87	21.041	6.841	26.118	1.00 53.17	0
	MOTA	418	ND2	ASN A	87	22.586	7.940	27.325	1.00 53.77	N
	MOTA	419	С	ASN A	87	23.722	8.028	22.735	1.00 50.39	С
	MOTA	420	0	ASN A	87	24.910	8.064	23.047	1.00 50.96	0
	MOTA	421	N	GLN A	88	23.303	8.032	21.474	1.00 49.81	N
10	MOTA	422	CA	GLN A	88	24.235	8.088	20.355	1.00 49.12	С
	MOTA	423	СВ	GLN A	88	24.552	6.676	19.859	1.00 49.66	С
	MOTA	424	CG	GLN A	88	25.641	6.620	18.804	1.00 52.17	С
	MOTA	425	CD	GLN A	88	25.868	5.217	18.273	1.00 54.04	С
	MOTA	426	OE1	GLN A	88	25.080	4.704	17.470	1.00 55.11	0
15	MOTA	427	NE2	GLN A	88	26.943	4.582	18.729	1.00 53.14	N
	MOTA	428	C	GLN A	88	23.640	8.901	19.212	1.00 47.52	С
	MOTA	429	0	GLN A	88	22.445	8.819	18.935	1.00 46.71	0
	ATOM	430	N	CYS A	89	24.482	9.690	18.554	1.00 46.02	N
	ATOM	431	CA	CYS A	89	24.038	10.504	17.435	1.00 44.64	С
20	ATOM	432	СВ	CYS A	89	24.929	11.736	17.271	1.00 45.12	С
	MOTA	433	SG	CYS A	89	24.884	12.871	18.685	1.00 48.12	S
	MOTA	434	С	CYS A	89	24.084	9.684	16.158	1.00 42.99	С
	ATOM	435	0	CYS A	89	25.144	9.207	15.750	1.00 42.55	0
	ATOM	436	N	GLU A	90	22.928	9.515	15.531	1.00 39.97	N
25	ATOM	437	CA	GLU A	90	22.856	8.763	14.295	1.00 38.16	С

	MOTA	438	СВ	GLU A	90	21.899	7.582	14.450	1.00 38.06	С
	MOTA	439	CG	GLU A	90	22.573	6.322	14.964	1.00 42.17	С
	MOTA	440	CD	GLU A	90	21.585	5.227	15.312	1.00 46.43	С
	MOTA	441	OE1	GLU A	90	20.657	4.981	14.511	1.00 46.83	0
5	MOTA	442	OE2	GLU A	90	21.745	4.604	16.389	1.00 50.51	0
	MOTA	443	С	GLU A	90	22.410	9.657	13.157	1.00 36.50	С
	MOTA	444	0	GLU A	90	21.854	10.729	13.372	1.00 35.05	0
	MOTA	445	N	THR A	91	22.678	9.214	11.940	1.00 34.79	N
	MOTA	446	CA	THR A	91	22.295	9.957	10.761	1.00 34.31	С
10	MOTA	447	СВ	THR A	91	23.500	10.641	10.100	1.00 34.34	С
	MOTA	448	OG1	THR A	91	23.799	11.852	10.805	1.00 30.72	0
	MOTA	449	CG2	THR A	91	23.202	10.958	8.642	1.00 33.63	С
	MOTA	450	С	THR A	91	21.668	8.991	9.787	1.00 34.16	С
	MOTA	451	0	THR A	91	22.191	7.907	9.545	1.00 35.05	0
15	MOTA	452	N	LYS A	92	20.530	9.393	9.240	1.00 33.69	N
	ATOM	453	CA	LYS A	92	19.810	8.571	8.289	1.00 33.19	С
	MOTA	454	СВ	LYS A	92	18.573	7.967	8.963	1.00 34.05	С
	MOTA	455	CG	LYS A	92	17.636	7.235	8.023	1.00 38.78	С
	MOTA	456	CD	LYS A	92	16.512	6.537	8.781	1.00 46.23	С
20	MOTA	457	CE	LYS A	92	15.775	5.552	7.877	1.00 48.21	С
	MOTA	458	NZ	LYS A	92	14.772	4.739	8.630	1.00 51.87	N
	MOTA	459	С	LYS A	92	19.395	9.419	7.094	1.00 31.39	С
	MOTA	460	0	LYS A	92	19.155	10.619	7.224	1.00 30.85	0
	MOTA	461	N	ILE A	93	19.323	8.786	5.930	1.00 29.87	N
25	MOTA	462	CA	ILE A	93	18.924	9.466	4.714	1.00 30.20	С

	MOTA	463	СВ	ILE A	93	20.005	9.352	3.620	1.00 29.62	С
	ATOM	464	CG1	ILE A	93	21.270	10.100	4.057	1.00 29.97	С
	MOTA	465	CD1	ILE A	93	22.423	9.998	3.066	1.00 34.73	С
	ATOM	466	CG2	ILE A	93	19.470	9.910	2.304	1.00 32.79	С
5	MOTA	467	С	ILE A	93	17.635	8.853	4.190	1.00 30.28	С
	MOTA	468	0	ILE A	93	17.567	7.647	3.943	1.00 31.07	0
	MOTA	469	N	MET A	94	16.609	9.686	4.049	1.00 28.71	N
	MOTA	470	CA	MET A	94	15.320	9.242	3.531	1.00 28.72	С
	MOTA	471	СВ	MET A	94	14.180	9.605	4.482	1.00 30.09	С
10	MOTA	472	CG	MET A	94	14.264	8.983	5.854	1.00 34.64	С
	MOTA	473	SD	MET A	94	12.774	9.336	6.815	1.00 47.69	S
	MOTA	474	CE	MET A	94	13.206	10.852	7.645	1.00 42.95	С
	MOTA	475	С	MET A	94	15.077	9.934	2.198	1.00 25.85	С
	MOTA	476	0	MET A	94	15.382	11.111	2.028	1.00 25.26	0
15	ATOM	477	N	VAL A	95	14.523	9.192	1,254	1.00 24.35	N
	ATOM	478	CA	VAL A	95	14.234	9.727	-0.067	1.00 22.51	С
	MOTA	479	СВ	VAL A	95	14.830	8.842	-1.183	1.00 22.28	С
	MOTA	480	CG1	VAL A	95	14.286	9.285	-2.523	1.00 22.94	С
	MOTA	481	CG2	VAL A	95	16.355	8.923	-1.171	1.00 24.47	С
20	MOTA	482	С	VAL A	95	12.737	9.812	-0.301	1.00 21.24	С
	ATOM	483	0	VAL A	95	12.052	8.791	-0.331	1.00 21.21	0
	MOTA	484	N	LEU A	96	12.232	11.033	-0.436	1.00 19.49	N
	MOTA	485	CA	LEU A	96	10.825	11.245	-0.729	1.00 21.14	С
	ATOM	486	СВ	LEU A	96	10.307	12.537	-0.088	1.00 19.27	С
25	MOTA	487	CG	LEU A	96	10.224	12.600	1.444	1.00 25.73	С

	MOTA	488	CD1	LEU A	96	9.644	13.948	1.877	1.00 26.81	С
	MOTA	489	CD2	LEU A	96	9.366	11.463	1.966	1.00 24.23	С
	MOTA	490	С	LEU A	96	10.728	11.344	-2.252	1.00 21.23	С
	MOTA	491	0	LEU A	96	11.129	12.355	-2.849	1.00 21.09	0
5	MOTA	492	N	GLN A	97	10.214	10.282	-2.873	1.00 20.36	N
	ATOM	493	CA	GLN A	97	10.063	10.223	-4.321	1.00 22.02	С
	MOTA	494	СВ	GLN A	97	9.916	8.771	-4.790	1.00 23.57	С
	MOTA	495	CG	GLN A	97	11.029	7.823	-4.391	1.00 24.69	С
	ATOM	496	CD	GLN A	97	12.313	8.111	-5.120	1.00 28.37	С
10	ATOM	497	OE1	GLN A	97	12.318	8.775	-6.155	1.00 28.08	0
	ATOM	498	NE2	GLN A	97	13.414	7.601	-4.592	1.00 31.31	N
	MOTA	499	С	GLN A	97	8.821	10.986	-4.758	1.00 21.48	С
	MOTA	500	0	GLN A	97	7.757	10.836	-4.164	1.00 21.39	0
	MOTA	501	N	PRO A	98	8.936	11.805	-5.815	1.00 22.84	N
15	MOTA	502	CA	PRO A	98	7.764	12.554	-6.273	1.00 23.56	С
	MOTA	503	СВ	PRO A	98	8.269	13.252	-7.540	1.00 22.35	С
	MOTA	504	CG	PRO A	98	9.343	12.347	-8.022	1.00 24.97	С
	MOTA	505	CD	PRO A	98	10.057	11.974	-6.749	1.00 20.37	С
	MOTA	506	С	PRO A	98	6.621	11.585	-6.543	1.00 25.12	С
20	MOTA	507	0	PRO A	98	6.847	10.473	-7.029	1.00 25.87	0
	MOTA	508	N	ALA A	99	5.401	12.001	-6.219	1.00 24.77	N
	MOTA	509	CA	ALA A	99	4.232	11.151	-6.410	1.00 26.15	С
	MOTA	510	СВ	ALA A	99	3.638	10.799	-5.053	1.00 24.62	С
	MOTA	511	С	ALA A	99	3.149	11.739	-7.323	1.00 27.20	С
25	ATOM	512	0	ALA A	99	1.973	11.766	-6.968	1.00 29.29	0

	MOTA	513	N	GLY A	100	3.547	12.223	-8.491	1.00 29.32	N
	ATOM	514	CA	GLY A	100	2.574	12.756	-9.435	1.00 30.75	С
	MOTA	515	С	GLY A	100	2.006	14.156	-9.255	1.00 30.83	С
	MOTA	516	0	GLY A	100	1.253	14.621	-10.118	1.00 32.00	0
5	MOTA	517	N	ALA A	101	2.337	14.832	-8.158	1.00 27.81	N
	ATOM	518	CA	ALA A	101	1.832	16.185	-7.931	1.00 27.20	С
	ATOM	519	СВ	ALA A	101	0.371	16.134	-7.475	1.00 27.02	С
	ATOM	520	С	ALA A	101	2.675	16.937	-6.904	1.00 25.78	С
	ATOM	521	Ο,	ALA A	101	3.185	16.348	-5.947	1.00 25.96	0
10	MOTA	522	N	PRO A 3	102	2.818	18.260	-7.082	1.00 26.56	N
	MOTA	523	CA	PRO A	102	3.615	19.056	-6.146	1.00 25.86	С
	ATOM	524	СВ	PRO A	102	3.415	20.487	-6.650	1.00 27.20	С
	MOTA	525	CG	PRO A	102	3.201	20.290	-8.120	1.00 29.43	С
	MOTA	526	CD	PRO A	102	2.255	19.118	-8.144	1.00 25.60	С
15	MOTA	527	С	PRO A	102	3.164	18.880	-4.703	1.00 24.43	С
	MOTA	528	0	PRO A	102	1.986	19.050	-4.386	1.00 25.38	0
	MOTA	529	N	GLY À	103	4.102	18.526	-3.831	1.00 22.57	N
	MOTA	530	CA	GLY A	103	3.764	18.351	-2.429	1.00 21.83	С
	MOTA	531	С	GLY A	103	3.324	16.944	-2.063	1.00 19.05	C
20	MOTA	532	0	GLY A	103	2.941	16.685	-0.920	1.00 20.94	0
	MOTA	533	N	HIS A	104	3.393	16.034	-3.028	1.00 18.00	N
	MOTA	534	CA	HIS A	104	3.016	14.644	-2.811	1.00 18.06	С
	MOTA	535	СВ	HIS A	104	1.845	14.277	-3.719	1.00 17.03	С
	MOTA	536	CG	HIS A	104	0.598	15.044	-3.417	1.00 21.85	С
25	MOTA	537	ND1	HIS A	104	-0.398	14.555	-2.599	1.00 19.71	N

	ATOM	538	CE1	HIS A	104	-1.329	15.478	-2.450	1.00 22.98	С
	ATOM	539	NE2	HIS A	104	-0.977	16.546	-3.144	1.00 16.26	N
	ATOM	540	CD2	HIS A	104	0.221	16.299	-3.761	1.00 18.82	С
	ATOM	541	С	HIS A	104	4.205	13.741	-3.094	1.00 16.96	С
5	ATOM	542	0	HIS A	104	4.812	13.815	-4.154	1.00 15.44	0
	MOTA	543	N	TYR A	105	4.521	12.873	-2.143	1.00 18.87	N
	ATOM	544	CA ·	TYR A	105	5.662	11.982	-2.284	1.00 18.50	С
	MOTA	545	СВ	TYR A	105	6.836	12.516	-1.456	1.00 20.43	С
	MOTA	546	CG	TYR A	105	7.115	13.996	-1.628	1.00 20.21	С
10	MOTA	547	CD1	TYR A	105	7.957	14.453	-2.645	1.00 18.18	С
	MOTA	548	CE1	TYR A	105	8.200	15.810	-2.821	1.00 20.31	С
	MOTA	549	CZ	TYR A	105	7.599	16.732	-1.975	1.00 20.71	С
	MOTA	550	OH	TYR A	105	7.845	18.072	-2.157	1.00 25.46	0
	MOTA	551	CE2	TYR A	105 .	6.756	16.310	-0.952	1.00 18.08	C
15	MOTA	552	CD2	TYR A	105.	6.521	14.941	-0.784	1.00 19.32	С
	MOTA	553	С	TYR A	105	5.349	10.579	-1.785	1.00 20.66	С
	MOTA	554	0	TYR A	105	4.355	10.350	-1.101	1.00 21.05	0
	MOTA	555	N	THR A	106	6.220	9.643	-2.136	1.00 21.73	N
	MOTA	556	CA	THR A	106	6.110	8.274	-1.666	1.00 25.27	С
20	MOTA	557	СВ	THR A	106	5.940	7.271	-2.825	1.00 24.65	С
	MOTA	558	OG1	THR A	106	7.009	7.427	-3.768	1.00 27.25	0
	MOTA	559	CG2	THR A	106	4.603	7.503	-3.531	1.00 26.01	С
	MOTA	560	С	THR A	106	7.425	8.017	-0.932	1.00 26.95	С
	MOTA	561	0	THR A	106	8.470	8.556	-1.304	1.00 25.88	0
25	MOTA	562	N	TYR A	107	7.375	7.209	0.118	1.00 30.17	N

	MOTA	563	CA	TYR A 1	07 8.570	6.916	0.896	1.00 33.45	С
	MOTA	564	СВ	TYR A 1	07 8.648	7.896	2.077	1.00 35.24	С
	MOTA	565	CG	TYR A 1	07 8.918	7.296	3.437	1.00 39.36	С
	MOTA	566	CD1	TYR A 1	07 10.146	6.707	3.736	1.00 43.99	С
5	ATOM	567	CE1	TYR A 1	07 10.401	6.182	4.999	1.00 47.50	С
	MOTA	568	CZ	TYR A 1	07 9.415	6.243	5.974	1.00 47.29	С
	MOTA	569	OH	TYR A 1	07 9.645	5.718	7.230	1.00 48.91	0
	MOTA	570	CE2	TYR A 10	07 8.190	6.823	5.693	1.00 44.53	С
	ATOM	571	CD2	TYR A 10	07 7.949	7.342	4.434	1.00 43.15	С
10	MOTA	572	С	TYR A 10	07 8.642	5.478	1.379	1.00 35.14	С
	MOTA	573	0	TYR A 10	07 7.682	4.943	1.924	1.00.35.69	0
	MOTA	574	N	SER A 10	08 9.800	4.864	1.172	1.00 37.81	N
	ATOM	575	CA	SER A 10	08 10.041	3.490	1.592	1.00 41.97	С
	MOTA	576	СВ	SER A 10	08 11.115	2.855	0.711	1.00 41.43	С
15	ATOM	577	Œ	SER A 10	08 11.572	1.645	1.282	1.00 44.65	0
	MOTA	578	С	SER A 1	08 10.500	3.455	3.047	1.00 43.76	С
	MOTA	579	0	SER A 10	08 11.583	3.940	3.372	1.00 45.52	0
	MOTA	580	N	SER A 1	09 9.684	2.868	3.918	1.00 46.53	N
	MOTA	581	CA	SER A 1	09 10.017	2.794	5.337	1.00 47.99	С
20	MOTA	582	СВ	SER A 1	09 8.740	2.876	6.173	1.00 48.18	С
	MOTA	583	Œ	SER A 1	09 9.052	2.943	7.552	1.00 48.31	0
	MOTA	584	С	SER A 1	09 10.799	1.536	5.720	1.00 49.24	С
	MOTA	585	0	SER A 1	09 10.870	0.568	4.957	1.00 51.51	0
	MOTA	586	N	SER A 1	12 9.886	-0.863	8.643	1.00 59.10	N
25	MOTA	587	CA	SER A 1	12 8.546	-1.374	8.383	1.00 58.71	С

	MOTA	588	CB	SER A 112	7.531	-0.229	8.378	1.00 59.10	С
	ATOM	589	Œ	SER A 112	6.241	-0.693	8.014	1.00 60.32	0
	ATOM	590	С	SER A 112	8.486	-2.096	7.046	1.00 57.85	С
	MOTA	591	0	SER A 112	7.722	-3.046	6.879	1.00 58.40	0
5	MOTA	592	N	GLY A 113	9.295	-1.639	6.096	1.00 56.85	N
	MOTA	593	CA	GLY A 113	9.301	-2.245	4.777	1.00 55.00	С
	MOTA	594	С	GLY A 113	8.170	-1.691	3.930	1.00 52.98	С
	ATOM	595	0	GLY A 113	8.254	-1.656	2.703	1.00 53.44	0
	MOTA	596	N	SER A 114	7.106	-1.257	4.595	1.00 50.93	N
10	MOTA	597	CA	SER A 114	5.940	-0.691	3.929	1.00 49.06	С
	MOTA	598	СВ	SER A 114	4.834	-0.441	4.955	1.00 49.17	С
	MOTA	599	Œ	SER A 114	5.283	0.435	5.980	1.00 50.92	0
	MOTA	600	С	SER A 114	6.268	0.620	3.222	1.00 46.96	C
	MOTA	601	0	SER A 114	7.323	1.211	3.443	1.00 47.26	0
15	MOTA	602	N	ILE A 115	5.355	1.062	2.364	1.00 44.72	N
	MOTA	603	CA	ILE A 115	5.508	2.315	1.636	1.00 42.22	C
	MOTA	604	СВ	ILE A 115	5.204	2.141	0.129	1.00 43.03	С
	ATOM	605	CG1	ILE A 115	6.307	1.316	-0.535	1.00 44.28	С
	ATOM	606	CD1	ILE A 115	7.674	1.972	-0.491	1.00 47.16	С
20	ATOM	607	CG2	ILE A 115	5.102	3.502	-0.552	1.00 43.16	С
	ATOM	608	С	ILE A 115	4.518	3.314	2.223	1.00 40.03	С
	MOTA	609	0	ILE A 115	3.449	2.932	2.705	1.00 39.69	0
	ATOM	610	N	HIS A 116	4.877	4.591	2.187	1.00 36.34	N
	ATOM	611	CA	HIS A 116	4.011	5.630	2.718	1.00 34.27	С
25	ATOM	612	СВ	HIS A 116	4.662	6.284	3.937	1.00 35.45	С

	MOTA	613	CG	HIS A	116	4.902	5.340	5.072	1.00 38.20	С
	MOTA	614	ND1	HIS A	116	5.654	5.683	6.176	1.00 41.13	N
	MOTA	615	CE1	HIS A	116	5.698	4.657	7.008	1.00 45.36	С
	MOTA	616	NE2	HIS A	116	5.001	3.664	6.485	1.00 40.45	N
5	MOTA	617	CD2	HIS A	116	4.492	4.066	5.273	1.00 40.93	С
	MOTA	618	С	HIS A	116	3.732	6.690	1.666	1.00 31.61	С
	MOTA	619	0	HIS A	116	4.542	6.914	0.768	1.00 30.20	0
	MOTA	620	N	SER A	117	2.572	7.325	1.781	1.00 28.75	N
	MOTA	621	CA	SER A	117	2.176	8.387	0.872	1.00 28.44	С
10	MOTA	622	СВ	SER A	117	0.785	8.119	0.302	1.00 26.28	С
	MOTA	623	œ	SER A	117	0.829	7.005 -	-0.566	1.00 32.61	0
	MOTA	624	С	SER A	117	2.179	9.667	1.692	1.00 26.02	С
	MOTA	625	0	SER A	117	1.323	9.860	2.556	1.00 26.95	0
	MOTA	626	N	VAL A	118	3.148	10.534	1.419	1.00 24.58	N
15	MOTA	627	CA	VAL A	118	3.299	11.785	2.161	1.00 22.06	С
	ATOM .	628	СВ	VAL A	118	4.796	12.044	2.497	1.00 23.75	С
	MOTA	629	CG1	VAL A	118	4.960	13.338	3.304	1.00 23.80	С
	MOTA	630	CG2	VAL A	118	5.349	10.867	3.279	1.00 25.01	С
	MOTA	631	С	VAL A	118	2.760	12.991	1.413	1.00 21.13	С
20	MOTA	632	0	VAL A	118	3.000	13.152	0.224	1.00 21.25	0
	MOTA	633	N	SER A	119	2.033	13.840	2.124	1.00 19.39	N
	MOTA	634	CA	SER A	119	1.495	15.046	1.522	1.00 19.65	С
	MOTA	635	СВ	SER A	119	-0.001	14.893	1.247	1.00 18.42	С
	MOTA	636	œ	SER A	119	-0.709	14.799	2.467	1.00 16.99	0
25	MOTA	637	С	SER A	119	1.720	16.222	2.471	1.00 20,44	С

	MOTA	638	0	SER A	119	1.734	16.060	3.694	1.00 20.31	0
	MOTA	639	N	VAL A	120	1.927	17.398	1.894	1.00 20.60	N
	MOTA	640	CA	VAL A	120	2.111	18.605	2.680	1.00 20.92	С
	MOTA	641	СВ	VAL A	120	2.911	19.665	1.909	1.00 21.47	С
5	MOTA	642	CG1	VAL A	120	3.008	20.934	2.747	1.00 21.53	С
	MOTA	643	CG2	VAL A	120	4.304	19.123	1.559	1.00 21.20	С
	MOTA	644	С	VAL A	120	0.713	19.159	2.942	1.00 19.42	С
	MOTA	645	0	VAL A	120	0.072	19.668	2.036	1.00 17.04	0
	MOTA	646	N	VAL A	121	0.238	19.040	4.174	1.00 18.30	N
10	MOTA	647	CA	VAL A	121	-1.090	19.542	4.519	1.00 17.84	С
	MOTA	648	СВ	VAL A	121	-1.487	19.110	5.942	1.00 17.08	С
	MOTA	649	CG1	VAL A	121	-2.886	19.650	6.297	1.00 15.35	С
	MOTA	650	CG2	VAL A	121	-1.429	17.607	6.050	1.00 18.80	С
	MOTA	651	С	VAL A	121	-1.105	21.069	4.444	1.00 17.06	С
15	MOTA	652	0	VAL A	121	-1.947	21.667	3.783	1.00 16.89	0
	ATOM	653	N	GLU A	122	-0.157	21.687	5.129	1.00 17.44	N
	MOTA	654	CA	GLU A	122	-0.048	23.139	5.152	1.00 19.43	С
	ATOM	655	СВ	GLU A	122	-0.945	23.704	6.254	1.00 17.85	С
	MOTA	656	CG	GLU A	122	-0.988	25.207	6.322	1.00 21.33	С
20	ATOM	657	CD	GLU A	122	-1.991	25.698	7.356	1.00 24.57	С
	ATOM	658	OE1	GLU A	122	-1.598	26.454	8.275	1.00 28.32	0
	ATOM	659	OE2	GLU A	122	-3.172	25.317	7.254	1.00 20.65	0
	ATOM	660	С	GLU A	122	1.405	23.465	5.460	1.00 18.95	С
	MOTA	661	0	GLU A	122	2.083	22.676	6.114	1.00 16.79	0
25	ATOM	662	N	ALA A	123	1.879	24.624	5.008	1.00 21.01	N

	ATOM	663	CA	ALA A 123	3.257	25.003	5.280	1.00 20.93	С
	MOTA	664	СВ	ALA A 123	3 4.202	24.042	4.559	1.00 20.51	С
	MOTA	665	С	ALA A 123	3.608	26.444	4.913	1.00 21.90	С
	MOTA	666	0	ALA A 123	3.009	27.036	4.021	1.00 23.30	0
5	ATOM	667	N	ASN A 124	4.584	26.989	5.638	1.00 21.77	N
	ATOM	668	CA	ASN A 124	5.126	28.333	5.433	1.00 20.98	С
	MOTA	669	СВ	ASN A 124	4.780	29.253	6.614	1.00 20.38	С
	ATOM	670	CG	ASN A 124	5.392	30.644	6.477	1.00 22.16	С
	ATOM	671	OD1	ASN A 124	6.495	30.809	5.951	1.00 22.44	0
10	ATOM	672	ND2	ASN A 124	4.683	31.650	6.971	1.00 26.85	N
	MOTA	673	С	ASN A 124	6.621	28.048	5.422	1.00 20.13	С
	MOTA	674	0	ASN A 124	7.211	27.813	6.466	1.00 19.09	0
	MOTA	675	N	TYR A 125	7.230	28.070	4.244	1.00 20.81	N
	ATOM ·	676	CA	TYR A 125	8.641	27.753	4.109	1.00 22.71	С
15	MOTA	677	СВ	TYR A 125	9.067	27.919	2.648	1.00 21.66	С
	ATOM	678	CG	TYR A 125	9.073	29.334	2.135	1.00 29.19	С
	MOTA	679	CD1	TYR A 125	10.112	30.200	2.459	1.00 31.37	С
•	MOTA	680	CE1	TYR A 125	10.161	31.485	1.956	1.00 36.25	С
	MOTA	681	CZ	TYR A 125	9.160	31.924	1.115	1.00 36.44	С
20	ATOM	682	OH	TYR A 125	9.251	33.193	0.597	1.00 39.33	0
	MOTA	683	CE2	TYR A 125	8.104	31.089	0.777	1.00 34.28	С
	MOTA	684	CD2	TYR A 125	8.067	29.798	1.290	1.00 30.61	С
	MOTA	685	С	TYR A 125	9.622	28.453	5.042	1.00 21.07	С
	MOTA	686	0	TYR A 125	5 10.748	27.986	5.203	1.00 22.41	0
25	ATOM	687	N	ASP A 126	9.211	29.549	5.673	1.00 21.85	N

	MOTA	688	CA	ASP A	126	10.098	30.251	6.603	1.00 22.62	С
	MOTA	689	СВ	ASP A	126	9.947	31.767	6.497	1.00 23.92	С
	MOTA	690	CG	ASP A	126	10.622	32.320	5.297	1.00 24.44	С
	MOTA	691	OD1	ASP A	126	11.604	31.692	4.863	1.00 29.05	0
5	MOTA	692	OD2	ASP A	126	10.179	33.376	4.803	1.00 24.13	0
	MOTA	693	С	ASP A	126	9.802	29.884	8.025	1.00 22.45	С
	MOTA	694	0	ASP A	126	10.487	30.334	8.946	1.00 22.45	0
	MOTA	695	N	GLU A	127	8.767	29.081	8.217	1.00 22.34	N
	MOTA	696	CA	GLU A	127	8.389	28.714	9.565	1.00 23.65	С
10	MOTA	697	СВ	GLU A	127	7.182	29.547	10.007	1.00 23.39	С
	MOTA	698	CG	GLU A	127	7.483	30.999	10.315	1.00 31.89	С
	MOTA	699	CD	GLU A	127	6.262	31.728	10.861	1.00 39.28	С
	MOTA	700	OE1	GLU A	127	5.611	31.186	11.783	1.00 42.40	0
	MOTA	701	OE2	GLU A	127	5.951	32.840	10.378	1.00 43.22	0
15	MOTA	702	С	GLU A	127	8.087	27.257	9.836	1.00 21.93	С
	MOTA	703	0	GLU A	127	8.627	26.694	10.778	1.00 22.92	0
	MOTA	704	N	TYR A	128	7.240	26.637	9.019	1.00 20.93	N
	MOTA	705	CA	TYR A	128	6.854	25.263	9.306	1.00 19.08	С
	MOTA	706	СВ	TYR A	128	5.827	25.276	10.441	1.00 19.89	С
20	MOTA	707	CG	TYR A	128	4.472	25.797	9.992	1.00 20.24	С
	MOTA	708	CD1	TYR A	128	3.520	24.934	9.447	1.00 20.50	С
	MOTA	709	CE1	TYR A	128	2.296	25.402	8.981	1.00 21.38	С
	MOTA	710	CZ	TYR A	128	2.008	26.754	9.056	1.00 26.85	С
	MOTA	711	OH	TYR A	128	0.792	27.207	8.594	1.00 28.12	0
25	MOTA	712	CE2	TYR A	128	2.934	27.644	9.593	1.00 26.44	С

	MOTA	713	CD2	TYR A	128	4.163	27.157	10.062	1.00 22.61	С
	MOTA	714	С	TYR A	128	6.267	24.492	8.140	1.00 19.35	С
	MOTA	715	0	TYR A	128	5.911	25.054	7.110	1.00 19.41	0
	MOTA	716	N	ALA A	129	6.153	23.183	8.335	1.00 19.30	N
5	MOTA	717	CA	ALA A	129	5.600	22.290	7.337	1.00 18.44	С
	MOTA	718	СВ	ALA A	129	6.715	21.673	6.493	1.00 19.76	С
	MOTA	719	С	ALA A	129	4.858	21.203	8.079	1.00 19.35	С
	MOTA	720	0	ALA A	129	5.440	20.519	8.923	1.00 19.02	0
	ATOM	721	N	LEU A	130	3.576	21.052	7.760	1.00 17.69	N
10	MOTA	722	CA	LEU A	130	2.720	20.050	8.384	1.00 17.03	С
	MOTA	723	СВ	LEU A	130	1.342	20.655	8.678	1.00 16.93	С
	MOTA	724	CG	LEU A	130	0.480	20.216	9.874	1.00 25.96	С
	ATOM	725	CD1	LEU A	130	-0.956	20.686	9.609	1.00 21.15	С
	MOTA	726	CD2	LEU A	130	0.516	18.687	10.081	1.00 26.45	С
15	MOTA	727	С	LEU A	130	2.582	18.932	7.354	1.00 17.75	C
	MOTA	728	0	LEU A	130	2.005	19.140	6.284	1.00 16.09	0
	MOTA	729	N	LEU A	131	3.128	17.754	7.657	1.00 17.47	N
	MOTA	730	CA	LEU A	131	3.040	16.640	6.727	1.00 16.94	С
	ATOM	731	СВ	LEU A	131	4.413	16.030	6.464	1.00 18.54	С
20	ATOM	732	CG	LEU A	131	5.595	16.886	5.995	1.00 21.25	С
	MOTA	733	CD1	LEU A	131	6.622	15.972	5.343	1.00 19.28	С
	MOTA	734	CD2	LEU A	131	5.153	17.941	5.021	1.00 20.56	С
	MOTA	735	С	LEU A	131	2.122	15.535	7.224	1.00 18.91	С
	MOTA	736	0	LEU A	131	2.019	15.274	8.429	1.00 18.27	0
25	MOTA	737	N	PHE A	132	1.444	14.892	6.286	1.00 18.52	N

	MOTA	738	CA	PHE A	132	0.569	13.784	6.628	1.00 20.01	С
	MOTA	739	СВ	PHE A	132	-0.876	14.046	6.214	1.00 20.97	С
	MOTA	740	CG	PHE A	132	-1.786	12.870	6.461	1.00 25.43	С
	MOTA	741	CD1	PHE A	132	-2.106	12.480	7.763	1.00 29.99	С
5	ATOM	742	CE1	PHE A	132	-2.904	11.359	8.003	1.00 30.06	С
	ATOM	743	CZ	PHE A	132	-3.391	10.616	6.933	1.00 29.29	С
	ATOM	744	CE2	PHE A	132	-3.083	10.993	5.629	1.00 30.24	С
	ATOM	745	CD2	PHE A	132	-2.282	12.119	5.397	1.00 27.73	С
	ATOM	746	С	PHE A	132	1.086	12.574	5.880	1.00 20.33	С
10	ATOM	747	0	PHE A	132	1.369	12.650	4.694	1.00 19.14	0
	ATOM	748	N	SER A	133	1.213	11.460	6.582	1.00 21.25	N
	ATOM	749	CA	SER A	133	1.698	10.238	5.973	1.00 24.44	C
	ATOM	750	СВ	SER A	133	3.077	9.916	6.536	1.00 22.99	С
	ATOM	751	œ	SER A	133	3.655	8.799	5.894	1.00 35.35	0
15	ATOM	752	С	SER A	133	0.724	9.092	6.247	1.00 25.26	С
	ATOM	753	0	SER A	133	0.270	8.895	7.375	1.00 24.85	0
	ATOM	754	N	ARG A	134	0.381	8.354	5.204	1.00 28.87	N
	ATOM	755	CA	ARG A	134	-0.525	7.231	5.352	1.00 32.47	С
	ATOM	756	СВ	ARG A	134	-1.888	7.530	4.701	1.00 32.31	С
20	MOTA	757	CG	ARG A	134	-1.834	8.152	3.316	1.00 37.53	С
	ATOM	758	CD	ARG A	134	-3.169	8.816	2.978	1.00 43.53	С
	MOTA	759	NE	ARG A	134	-3.169	9.553	1.712	1.00 44.76	N
	MOTA	760	CZ	ARG A	134	-3.163	8.983	0.511	1.00 44.99	С
	ATOM	761	NH1	ARG A	134	-3.147	7.661	0.405	1.00 46.67	N
25	MOTA	762	NH2	ARG A	134	-3.215	9.732	-0.587	1.00 42.69	N

	MOTA	763	С	ARG A	134	0.105	5.994	4.746	1.00 35.05	С
	MOTA	764	0	ARG A	134	0.695	6.038	3.661	1.00 32.09	0
	ATOM	765	N	GLY A	135	0.003	4.897	5.484	1.00 38.13	N
	MOTA	766	CA	GLY A	135	0.556	3.640	5.033	1.00 43.65	С
5	MOTA	767	С	GLY A	135	-0.446	2.537	5.290	1.00 48.0	1 C
	MOTA	768	0	GLY A	135	-1.472	2.760	5.937	1.00 47.4	9 0
	MOTA	769	N	THR A	136	-0.162	1.344	4.783	1.00 51.7	3 N
	MOTA	770	CA	THR A	136	-1.070	0.219	4.969	1.00 55.5	9 C
	MOTA	771	СВ	THR A	136	-2.315	0.358	4.067	1.00 55.8	4 C
10	MOTA	772	Œ1	THR A	136	-2.924	1.634	4.284	1.00 58.7	8 0
	MOTA	773	CG2	THR A	136	-3.331	-0.725	4.386	1.00 56.7	6 C
	MOTA	774	С	THR A	136	-0.382	-1.094	4.636	1.00 56.8	9 C
	MOTA	775	0	THR A	136	-0.138	-1.392	3.470	1.00 57.0	1 0
	MOTA	776	N	LYS A	137	-0.075	-1.875	5.667	1.00 59.2	8 N
15	MOTA	777	CA	LYS A	137	0.580	-3.162	5.483	1.00 61.56	С
	MOTA	778	СВ	LYS A	137	0.971	-3.763	6.834	1.00 61.96	С
	MOTA	779	CG	LYS A	137	1.531	-2.777	7.849	1.00 63.75	С
	MOTA	780	CD	LYS A	137	1.803	-3.478	9.176	1.00 66.26	С
	MOTA	781	CE	LYS A	137	2.248	-2.499	10.252	1.00 66.38	С
20	MOTA	782	NZ	LYS A	137	2.545	-3.196	11.536	1.00 66.02	N
	MOTA	783	С	LYS A	137	-0.411	-4.096	4.800	1.00 62.3	6 C
	MOTA	784	0	LYS A	137	-0.041	-5.159	4.300	1.00 63.0	4 0
	MOTA	785	. N	GLY A	138	-1.678	-3.691	4.791	1.00 63.0	5 N
	MOTA	786	CA	GLY A	138	-2.714	-4.501	4.176	1.00 63.3	5 C
25	ATOM	787	С	GLY A	138	-4.104	-4.069	4.610	1.00 63.6	1 C

	MOTA	788	0	GLY A	138	-4.231	-3.171	5.435	1.00	64.06	0
	ATOM	789	N	PRO A	139	-5.168	-4.690	4.079	1.00	63.70	N
	MOTA	790	CA	PRO A	139	-6.555	-4.348	4.430	1.00	63.74	С
	ATOM	791	СВ	PRO A	139	-7.369	-5.364	3.639	1.00	63.65	С
5	ATOM	792	CG	PRO A	139	-6.503	-5.603	2.422	1.00	64.02	С
	ATOM	793	CD	PRO A	139	-5.125	-5.708	3.016	1.00	63.81	С
	ATOM	794	С	PRO A	139	-6.833	-4.419	5.935	1.00	63.55	С
	MOTA	795	0	PRO A	139	-7.057	-5.490	6.494	1.00	63.71	0
	ATOM	796	N	GLY A	140	-6.822	-3.261	6.584	1.00	63.03	N
10	ATOM	797	CA	GLY A	140	-7.059	-3.199	8.018	1.00	62.01	С
	MOTA	798	С	GLY A	140	-5.787	-2.914	8.800	1.00	60.77	С
	ATOM T	799	0	GLY A	140	-5.827	-2.660	10.004	1.00	60.90	0
	MOTA	800	N	GLN A	141	-4.653	-2.947	8.112	1.00	59.05	N
	MOTA	801	CA ·	GLN A	141	-3.373	-2.694	8.752	1.00	57.46	С
15	ATOM	802	СВ	GLN A	141	-2.398	-3.809	8.370	1.00	57.71	С
	MOTA	803	CG	GLN A	141	-3.090	-5.178	8.473	1.00	58.74	С
	MOTA	804	CD	GLN A	141	-2.189	-6.355	8.151	1.00	59.31	С
	ATOM	805	OE1	GLN A	141	-1.552	-6.402	7.093	1.00	58.75	0
	MOTA	806	NE2	GLN A	141	-2.141	-7.323	9.063	1.00	59.08	N
20	ATOM	807	С	GLN A	141	-2.882	-1.323	8.304	1.00	55.66	С
	ATOM	808	0	GLN A	141	-1.699	-1.125	8.029	1.00	55.85	0
	ATOM	809	N	ASN A	142	-3.825	-0.383	8.247	1.00	53.33	N
	ATOM	810	CA	ASN A	142	-3.570	0.998	7.836	1.00	51.55	С
	ATOM	811	СВ	ASN A	142	-4.857	1.649	7.316	1.00	51.60	С
25	ATOM	812	CG	ASN A	142	-5.936	0.642	6.973	1.00	53.89	С

	MOTA	813	OD1	ASN A 14	42 -	7.123	0.905	7.172	1.00	53.86	0
	ATOM	814	ND2	ASN A 1	42 -!	5.534	-0.511	6.442	1.00	58.03	N
	MOTA	815	С	ASN A 14	42 -:	3.069	1.843	9.005	1.00	49.32	С
	MOTA	816	0	ASN A 14	42 -3	3.655	1.828	10.081	1.00	49.92	0
5	MOTA	817	N	PHE A 14	43 -:	1.995	2.593	8.787	1.00	46.30	N
	MOTA	818	CA	PHE A 14	43 -	1.459	3.458	9.829	1.00	43.59	С
	MOTA	819	СВ	PHE A 14	43 -0	0.089	2.953	10.285	1.00	44.54	С
	MOTA	820	CG	PHE A 14	43 1	.056	3.775	9.777	1.00 4	8.28	С
	MOTA	821	CD1	PHE A 14	43 1	.621	4.764	10.573	1.00 5	1.58	С
10	MOTA	822	CE1	PHE A 14	43 2	.650	5.570	10.093	1.00 5	4.13	С
	MOTA	823	CZ	PHE A 14	43 3	.121	5.388	8.807	1.00 5	2.35	С
	MOTA	824	CE2	PHE A 14	43 2	.566	4.400	8.001	1.00 5	3.51	С
	MOTA	825	CD2	PHE A 14	43 1	.538	3.597	8.490	1.00 5	0.84	С
	MOTA	826	C	PHE A 14	43 –:	1.350	4.886	9.292	1.00	40.43	С
15	MOTA	827	0	PHE A 14	43 -1	1.134	5.094	8.103	1.00	37.35	0
	MOTA	828	N	ARG A 14	44 -1	1.509	5.864	10.176	1.00	37.08	N
	MOTA	829	CA	ARG A 14	44 -1	1.441	7.267	9.796	1.00	34.89	С
	MOTA	830	СВ	ARG A 14	44 -2	2.833	7.897	9.918	1.00	35.73	С
	ATOM	831	CG	ARG A 14	44 -3	3.816	7.364	8.872	1.00	39.13	С
20	MOTA	832	CD	ARG A 14	44 -	5.240	7.894	9.029	1.00	46.28	С
	ATOM	833	NE	ARG A 14	44 -	6.006	7.160	10.035	1.00	49.14	N
	ATOM	834	CZ	ARG A 14	44 -!	5.866	7.314	11.348	1.00	52.48	С
	ATOM	835	NH1	ARG A 14	44 -	4.988	8.182	11.829	1.00	54.40	N
	ATOM	836	NH2	ARG A 14	44 -	6.608	6.599	12.183	1.00	54.82	N
25	ATOM	837	С	ARG A 1	44 -	0.435	8.017	10.666	1.00	32.66	С

	ATOM	838	0	ARG A	144	-0.278	7.712	11.846	1.00 30.70	0
	MOTA	839	N	MET A	145	0.259	8.988	10.084	1.00 28.76	N
	MOTA	840	CA	MET A	145	1.232	9.749	10.850	1.00 27.41	С
	MOTA	841	СВ	MET A	145	2.612	9.099	10.747	1.00 27.81	С
5	MOTA	842	CG	MET A	145	3.715	9.914	11.408	1.00 30.09	С
	MOTA	843	SD	MET A	145	5.311	9.070	11.470	1.00 35.29	s
	MOTA	844	CE	MET A	145	5.842	9.159	9.789	1.00 30.22	С
	MOTA	845	С	MET A	145	1.336	11.214	10.452	1.00 26.47	С
	MOTA	846	0	MET A	145	1.565	11.543	9.285	1.00 27.37	0
10	MOTA	847	N	ALA A	146	1.178	12.086	11.442	1.00 24.27	N
	MOTA	848	CA	ALA A	146	1.267	13.527	11.242	1.00 22.72	С
	MOTA	849	СВ	ALA A	146	0.161	14.223	12.004	1.00 23.19	С
	MOTA	850	С	ALA A	146	2.633	13.998	11.743	1.00 21.85	С
	MOTA	851	0	ALA A	146	3.047	13.670	12.860	1.00 20.76	0
15	MOTA	852	N	THR A	147	3.332	14.765	10.914	1.00 21.71	N
	MOTA	853	CA	THR A	147	4.652	15.261	11.281	1.00 20.82	С
	MOTA	854	СВ	THR A	147	5.747	14.641	10.388	1.00 22.25	С
	MOTA	855	OG1	THR A	147	5.541	13.224	10.287	1.00 23.42	0
	MOTA	856	CG2	THR A	147	7.125	14.910	10.977	1.00 22.09	С
20	MOTA	857	С	THR A	147	4.738	16.776	11.143	1.00 20.34	С
	MOTA	858	0	THR A	147	4.339	17.342	10.125	1.00 19.27	0
	MOTA	859	N	LEU A	148	5.269	17.430	12.170	1.00 19.28	N
	MOTA	860	CA	LEU A	148	5.409	18.878	12.137	1.00 19.58	С
	MOTA	861	СВ	LEU A	148	4.675	19.516	13.317	1.00 21.33	С
25	MOTA	862	CG	LEU A	148	4.786	21.045	13.445	1.00 20.43	С

	ATOM	863	CD1	LEU A	148	4.224	21.747	12.219	1.00 22.47	С
	MOTA	864	CD2	LEU A	148	4.026	21.472	14.671	1.00 24.32	С
	MOTA.	865	С	LEU A	148	6.877	19.289	12.155	1.00 19.02	С
	MOTA	866	0	LEU A	148	7.605	19.046	13.127	1.00 18.11	0
5	MOTA	867	N	TYR A	149	7.308	19.887	11.051	1.00 19.53	N
	MOTA	868	CA	TYR A	149	8.671	20.378	10.923	1.00 19.40	С
	MOTA	869	СВ	TYR A	149	9.206	20.132	9.518	1.00 19.80	С
	MOTA	870	CG	TYR A	149	9.662	18.712	9.281	1.00 22.86	С
	ATOM	871	CD1	TYR A	149	10.829	18.219	9.873	1.00 24.22	С
10	MOTA	872	CE1	TYR A	149	11.236	16.889	9.672	1.00 25.00	С
	MOTA	873	CZ	TYR A	149	10.464	16.058	8.877	1.00 26.70	С
	MOTA	874	OH	TYR A	149	10.819	14.742	8.693	1.00 36.47	0
	MOTA	875	CE2	TYR A	149	9.305	16.531	8.280	1.00 27.17	С
	MOTA	876	CD2	TYR A	149	8.910	17.844	8.482	1.00 25.06	C
15	MOTA	877	C .	TYR A	149	8.658	21.872	11.208	1.00 19.85	C
	MOTA	878	0	TYR A	149	7.672	22.562	10.938	1.00 18.56	0
	MOTA	879	N	SER A	150	9.764	22.363	11.750	1.00 19.94	N
	MOTA	880	CA	SER A	150	9.903	23.764	12.102	1.00 20.50	С
	MOTA	881	СВ	SER A	150	9.704	23.915	13.615	1.00 21.21	С
20	MOTA	882	Œ	SER A	150	9.899	25.250	14.047	1.00 22.73	0
	ATOM	883	С	SER A	150	11.282	24.302	11.701	1.00 20.46	С
	ATOM	884	0	SER A	150	·12.292	23.593	11.778	1.00 18.66	0
	ATOM	885	N	ARG A	151	11.319	25.556	11.261	1.00 21.36	N
	ATOM	886	CA	ARG A	151	12.587	26.164	10.878	1.00 22.36	С
25	ATOM	887	СВ	ARG A	151	12.355	27.467	10.102	1.00 21.14	С

	MOTA	888	CG	ARG A	151	11.888	27.250	8.673	1.00 2	22.84	С
	MOTA	889	CD	ARG A	151	12.914	26.442	7.873	1.00	19.77	С
	MOTA	890	NE	ARG A	151	12.582	26.404	6.448	1.00 2	24.92	N
	MOTA	891	CZ	ARG A	151	13.337	25.841	5.511	1.00 2	20.64	С
5	MOTA	892	NH1	ARG A	151	14.479	25.258	5.836	1.00 2	22.01	N
	MOTA	893	NH2	ARG A	151	12.948	25.869	4.243	1.00 2	21.20	N
	MOTA	894	С	ARG A	151	13.387	26.437	12.145	1.00 2	23.99	С
	ATOM	895	0	ARG A	151	14.615	26.506	12.115	1.00 2	24.51	0
	ATOM	896	N	THR A	152	12.676	26.578	13.258	1.00 2	24.32	N
10	MOTA	897	CA	THR A	152	13.305	26.832	14.548	1.00 2	26.33	С
	MOTA	898	СВ	THR A	152	12.765	28.120	15.185	1.00 2	27.25	С
	MOTA	899	OG1	THR A	152	11.347	27.997	15.378	1.00 2	25.22	0
	MOTA	900	CG2	THR A	152	13.063	29.327	14.295	1.00 2	25.83	С
	MOTA	901	С	THR A	152	13.047	25.687	15.528	1.00 2	27.69	С
15	ATOM	902	0	THR A	152	12.090	24.928	15.372	1.00 2	26.48	0
	MOTA	903	N	GLN A	153	13.906	25.576	16.536	1.00 2	28.98	N
	MOTA	904	CA	GLN A	153	13.776	24.538	17.551	1.00	30.08	С
	ATOM	905	СВ	GLN A	153	15.090	24.396	18.329	1.00 2	29.88	С
	MOTA	906	CG	GLN A	153	16.182	23.642	17.582	1.00	32.02	С
20	MOTA	907	CD	GLN A	153	17.493	23.587	18.347	1.00	35.05	С
	MOTA	908	OE1	GLN A	153	18.400	24.373	18.099	1.00	36.34	0
	MOTA	909	NE2	GLN A	153	17.591	22.658	19.289	1.00	36.94	N
	MOTA	910	С	GLN A	153	12.629	24.848	18.513	1.00	30.99	С
	MOTA	911	0	GLN A	153	12.158	23.972	19.236	1.00	31.14	0
25	MOTA	912	N	THR A	154	12.187	26.100	18.517	1.00	33.09	N

	MOTA	913	CA	THR A	154	11.095	26.526	19.382	1.00 35.59	С
	ATOM	914	СВ	THR A	154	11.334	27.944	19.923	1.00 35.74	С
	ATOM	915	Œ1	THR A	154	12.404	27.905	20.870	1.00 40.23	0
	MOTA	916	CG2	THR A	154	10.090	28.481	20.608	1.00 36.81	С
5	ATOM	917	С	THR A	154	9.788	26.492	18.611	1.00 36.05	С
	ATOM	918	0	THR A	154	9.737	26.835	17.431	1.00 36.13	0
	ATOM	919	N	LEU A	155	8.724	26.083	19.288	1.00 37.13	N _.
	ATOM	920	CA	LEU A	155	7.422	25.975	18.648	1.00 38.42	С
	MOTA	921	СВ	LEU A	155	6.965	24.516	18.714	1.00 37.88	С
10	ATOM	922	CG	LEU A	155	6.062	23.916	17.638	1.00 39.67	С
	ATOM	923	CD1	LEU A	155	6.706	24.033	16.262	1.00 35.31	С
	MOTA	924	CD2	LEU A	155	5.816	22.456	17.984	1.00 38.75	С
	MOTA	925	С	LEU A	155	6.405	26.878	19.337	1.00 39.23	С
	MOTA	926	0	LEU A	155	6.264	26.841	20.561	1.00 39.64	0
15	ATOM	927	N	LYS A	156	5.708	27.697	18.553	1.00 39.22	N
	ATOM	928	CA	LYS A	156	4.690	28.589	19.102	1.00 39.41	С
	ATOM	929	СВ	LYS A	156	4.362	29.716	18.120	1.00 39.99	С
	ATOM	930	CG	LYS A	156	5.469	30.741	17.955	1.00 41.50	С
	ATOM	931	CD	LYS A	156	5.064	31.818	16.971	1.00 44.94	С
20	ATOM	932	CE	LYS A	156	6.165	32.854	16.791	1.00 46.38	С
	ATOM	933	NZ	LYS A	156	5.773	33.857	15.764	1.00 47.77	N
	ATOM	934	С	LYS A	156	3.426	27.798	19.398	1.00 39.33	С
	ATOM	935	0	LYS A	156	3.010	26.953	18.602	1.00 37.57	0
	ATOM	936	N	ASP A	157	2.815	28.082	20.544	1.00 39.71	N
25	ATOM	937	CA	ASP A	157	1.603	27.389	20.961	1.00 39.53	С

	MOTA	938	СВ	ASP A	157	1.028	28.063	22.208	1.00 41.01	С
	ATOM	939	CG	ASP A	157	2.033	28.131	23.343	1.00 43.20	С
	ATOM	940	OD1	ASP A	157	3.036	28.863	23.205	1.00 47.67	0
	ATOM	941	OD2	ASP A	157	1.828	27.445	24.368	1.00 46.90	0
5	ATOM	942	С	ASP A	157	0.538	27.310	19.868	1.00 38.74	С
	ATOM	943	0	ASP A	157	-0.132	26.287	19.720	1.00 37.95	0
	ATOM	944	N	GLU A	158	0.384	28.383	19.101	1.00 37.72	N
	ATOM	945	CA	GLU A	158	-0.609	28.398	18.033	1.00 37.05	С
	ATOM	946	СВ	GLU A	158	-0.614	29.752	17.321	1.00 37.76	С
10	ATOM	947	CG	GLU A	158	-0.463	30.954	18.243	1.00 41.78	С
	ATOM	948	CD	GLU A	158	0.977	31.198	18.656	1.00 46.94	С
	ATOM	949	OE1	GLU A	158	1.798	31.525	17.772	1.00 50.90	0
	ATOM	950	OE2	GLU A	158	1.292	31.063	19.859	1.00 49.28	0
	ATOM	951	С	GLU A	158	-0.294	27.301	17.024	1.00 35.99	С
15	ATOM	952	0	GLU A	158	-1.187	26.761	16.378	1.00 34.01	0
	ATOM	953	N	LEU A	159	0.990	26.981	16.895	1.00 35.06	N
	MOTA	954	CA	LEU A	159	1.437	25.948	15.969	1.00 32.93	С
	ATOM	955	СВ	LEU A	159	2.924	26.130	15.666	1.00 33.58	С
	ATOM	956	CG	LEU A	159	3.403	25.650	14.295	1.00 32.35	С
20	ATOM	957	CD1	LEU A	159	2.543	26.264	13.202	1.00 35.68	С
	ATOM	958	CD2	LEU A	159	4.857	26.040	14.104	1.00 33.17	С
	MOTA	959	С	LEU A	159	1.182	24.588	16.600	1.00 31.25	С
	ATOM	960	0	LEU A	159	0.851	23.622	15.914	1.00 29.46	0
	MOTA	961	N	LYS A	160	1.330	24.518	17.918	1.00 29.57	N
25	MOTA	962	CA	LYS A	160	1.077	23.276	18.633	1.00 29.07	С

	MOTA	963	СВ	LYS A 16	0 1.448	23.410	20.114	1.00 29.49	С
	ATOM	964	CG	LYS A 16	0 2.938	23.535	20.410	1.00 31.30	С
	ATOM	965	CD	LYS A 16	3.195	23.359	21.902	1.00 32.92	С
	MOTA	966	CE	LYS A 16	0 4.671	23.470	22.231	1.00 39.23	С
5	ATOM	967	NZ	LYS A 16	0 4.974	23.172	23.664	1.00 42.27	N
	MOTA	968	С	LYS A 16	0 -0.408	22.937	18.514	1.00 28.08	С
	ATOM	969	0	LYS A 16	0 -0.779	21.773	18.330	1.00 27.38	0
	MOTA	970	N	GLU A 16	1 -1.254	23.959	18.605	1.00 27.07	N
	ATOM	971	CA	GLU A 16:	1 -2.695	23.762	18.517	1.00 27.31	С
10	MOTA	972	СВ	GLU A 16:	1 -3.439	25.064	18.830	1.00 28.93	С
	MOTA	973	CG	GLU A 16:	1 -3.159	25.662	20.201	1.00 32.16	С
	MOTA	974	CD	GLU A 16:	1 -4.254	26.629	20.639	1.00 38.78	С
•	ATOM	975	OE1	GLU A 16	1 -4.944	27.191	19.758	1.00 39.33	0
	MOTA	976	OE2	GLU A 16	1 -4.422	26.831	21.864	1.00 43.12	0
15	MOTA	977	С	GLU A 16	1 -3.100	23.270	17.134	1.00 26.18	С
	MOTA	978	0	GLU A 16	1 -3.950	22.383	16.992	1.00 26.11	0
	MOTA	979	N	LYS A 16	2 -2.492	23.848	16.109	1.00 24.62	N
	MOTA	980	CA	LYS A 16	2 -2.794	23.440	14.742	1.00 24.49	С
•	MOTA	981	СВ	LYS A 16	2 -1.989	24.293	13.751	1.00 24.75	С
20	MOTA	982	CG	LYS A 16	2 -2.266	23.987	12.292	1.00 26.25	С
	ATOM	983	CD	LYS A 16	2 -1.240	24.660	11.369	1.00 30.87	С
	ATOM	984	CE	LYS A 16	2 -1.321	26.180	11.412	1.00 29.17	С
	ATOM	985	NZ	LYS A 16	2 -2.572	26.713	10.801	1.00 30.29	N
	MOTA	986	С	LYS A 16	2 -2.454	21.957	14.564	1.00 23.72	С
25	MOTA	987	0	LYS A 16	2 -3.219	21.198	13.973	1.00 21.42	0

	MOTA	988	N	PHE A 163	-1.304	21.545	15.090	1.00 23.78	N
	ATOM	989	CA	PHE A 163	-0.867	20.155	14.974	1.00 23.17	С
	ATOM	990	СВ	PHE A 163	0.539	20.007	15.560	1.00 21.98	С
	MOTA	991	CG	PHE A 163	1.159	18.664	15.306	1.00 21.44	С
5	MOTA	992	CD1	PHE A 163	1.376	18.219	14.008	1.00 17.30	С
	MOTA	993	CE1	PHE A 163	1.953	16.985	13.772	1.00 18.89	С
	MOTA	994	CZ	PHE A 163	2.323	16.173	14.841	1.00 22.89	С
	MOTA	995	CE2	PHE A 163	2.111	16.602	16.138	1.00 23.52	C
	MOTA	996	CD2	PHE A 163	1.531	17.844	16.367	1.00 21.36	С
10	MOTA	997	С	PHE A 163	-1.842	19.218	15.699	1.00 23.35	С
	MOTA	998	0	PHE A 163	-2.291	18.213	15.139	1.00 24.15	0
	MOTA	999	N	THR A 164	-2.161	19.550	16.946	1.00 26.31	N
	MOTA	1000	CA	THR A 164	-3.097	7 18.761	L 17.743	3 1.00 27.06	С
	MOTA	1001	СВ	THR A 164	-3.287	7 19.389	9 19.139	1.00 26.63	С
15	MOTA	1002	OG1	THR A 164	-2.023	3 19.415	5 19.817	7 1.00 29.13	0
	MOTA	1003	CG2	2 THR A 164	-4.288	3 18.585	5 19.969	9 1.00 28.94	С
	MOTA	1004	С	THR A 164	-4.447	7 18.683	L 17.034	1.00 26.30	С
	MOTA	1005	0	THR A 164	-5.045	5 17.609	9 16.937	7 1.00 27.05	0
	MOTA	1006	N	THR A 165	-4.917	7 19.81	7 16.534	1 1.00 26.32	N
20	MOTA	1007	CA	THR A 165	-6.191	19.86	5 15.813	3 1.00 28.31	С
	MOTA	1008	СВ	THR A 165	-6.511	L 21.294	15.320	1.00 27.79	С
	MOTA	1009	OG1	THR A 165	-6.587	7 22.184	16.44	l 1.00 31.94	0
	ATOM	1010	CG2	2 THR A 165	-7.834	1 21.316	5 14.579	9 1.00 31.80	С
	MOTA	1011	С	THR A 165	-6.178	3 18.94	7 14.58	5 1.00 26.45	С
25	ATOM	1012	0	THR A 165	-7.073	3 18.108	3 14.40	5 1.00 25.73	0

	MOTA	1013	N	PHE A 166	-5.172	19.110	13.731	1.00 25.04	N
	MOTA	1014	CA	PHE A 166	-5.087	18.278	12.540	1.00 23.74	С
	MOTA	1015	СВ	PHE A 166	-3.878	18.635	11.684	1.00 22.45	С
	MOTA	1016	CG	PHE A 166	-3.663	17.672	10.542	1.00 23.00	С
5	MOTA	1017	CD1	PHE A 166	-4.578	17.605	9.492	1.00 17.54	С
	ATOM	1018	CE1	PHE A 166	-4.408	16.709	8.451	1.00 15.87	С
	MOTA	1019	CZ	PHE A 166	-3.305	15.859	8.437	1.00 15.82	С
	MOTA	1020	CE2	PHE A 166	-2.380	15.912	.9.481	1.00 20.54	С
	MOTA	1021	CD2	PHE A 166	-2.564	16.818	10.524	1.00 23.28	С
10	MOTA	1022	С	PHE A 166	-4.986	16.808	12.909	1.00 23.55	С
	MOTA	1023	0	PHE A 166	-5.601	15.954	12.266	1.00 24.15	0
	ATOM	1024	N	SER A 167	-4.196	16.522	13.937	1.00 24.73	N
	ATOM	1025	CA	SER A 167	-3.994	15.156	14.392	1.00 25.60	С
	ATOM	1026	СВ	SER A 167	-2.978	15.132	15.541	1.00 26.04	С
15	MOTA	1027	Œ	SER A 167	-1.734	15.675	15.130	1.00 23.06	0
	ATOM	1028	С	SER A 167	-5.299	14.516	14.853	1.00 27.30	С
	MOTA	1029	0	SER A 167	-5.573	13.349	14.561	1.00 27.39	0
	MOTA	1030	N	LYS A 168	-6.105	15.279	15.580	1.00 28.09	N
	MOTA	1031	CA	LYS A 168	-7.364	14.753	16.070	1.00 28.24	С
20	MOTA	1032	СВ	LYS A 168	-7.915	15.668	17.167	1.00 28.85	С
	ATOM	1033	CG	LYS A 168	-7.015	15.656	18.404	1.00 29.37	С
	MOTA	1034	CD	LYS A 168	-7.628	16.376	19.581	1.00 31.71	С
	MOTA	1035	CE	LYS A 168	-6.778	16.162	20.821	1.00 31.05	С
	MOTA	1036	NZ	LYS A 168	-7.424	16.689	22.059	1.00 33.19	N
25	MOTA	1037	С	LYS A 168	-8.346	14.587	14.924	1.00 28.80	С

	MOTA	1038	0	LYS A 168	-9.116	13.632	14.896	1.00 28.47	0
	MOTA	1039	N	ALA A 169	-8.292	15.499	13.959	1.00 29.16	N
	MOTA	1040	CA	ALA A 169	-9.172	15.430	12.798	1.00 30.36	С
	MOTA	1041	СВ	ALA A 169	-9.021	16.681	11.949	1.00 29.30	С
5	MOTA	1042	С	ALA A 169	-8.819	14.194	11.978	1.00 31.34	С
	MOTA	1043	0	ALA A 169	-9.472	13.880	10.988	1.00 32.11	0
	MOTA	1044	N	GLN A 170	-7.774	13.493	12.394	1.00 32.26	N
	MOTA	1045	CA	GLN A 170	-7.347	12.295	11.689	1.00 32.22	С
	MOTA	1046	СВ	GLN A 170	-5.871	12.412	11.301	1.00 31.66	С
10	MOTA	1047	CG	GLN A 170	-5.570	13.544	10.319	1.00 31.19	С
	MOTA	1048	CD	GLN A 170	-6.351	13.407	9.018	1.00 30.95	С
	MOTA	1049	OE1	GLN A 170	-6.326	12.355	8.383	1.00 26.84	0
	MOTA	1050	NE2	GLN A 170	-7.042	14.470	8.618	1.00 28.03	N
	MOTA	1051	С	GLN A 170	-7.570	11.048	12.539	1.00 33.04	С
15	MOTA	1052	0	GLN A 170	-7.102	9.961	12.203	1.00 33.24	0
	MOTA	1053	N	GLY A 171	-8.291	11.211	13.641	1.00 34.12	N
	MOTA	1054	CA	GLY A 171	-8.565	10.082	14.509	1.00 36.19	С
	MOTA	1055	С	GLY A 171	-7.421	9.742	15.445	1.00 37.27	С
	MOTA	1056	0	GLY A 171	-7.243	8.584	15.823	1.00 37.31	0
20	ATOM	1057	N	LEU A 172	-6.633	10.747	15.812	1.00 38.22	N
•	MOTA	1058	CA	LEU A 172	-5.518	10.537	16.721	1.00 38.52	С
	MOTA	1059	СВ	LEU A 172	-4.226	11.119	16.135	1.00 37.99	С
	ATOM	1060	CG	LEU A 172	-3.719	10.490	14.825	1.00 38.07	С
	MOTA	1061	CD1	LEU A 172	-2.419	11.158	14.387	1.00 34.97	С
25	ATOM	1062	CD2	LEU A 172	-3.496	8.998	15.018	1.00 38.27	С

	MOTA	1063	С	LEU A 172	-5.843	11.204	18.049	1.00 39.21	С
	ATOM	1064	0	LEU A 172	-6.293	12.348	18.090	1.00 40.20	0
	MOTA	1065	N	THR A 173	-5.627	10.480	19.138	1.00 39.94	N
	ATOM	1066	CA	THR A 173	-5.893	11.011	20.467	1.00 40.68	С
5	ATOM	1067	СВ	THR A 173	-6.269	9.884	21.436	1.00 40.28	С
	MOTA .	1068	OG1	THR A 173	-5.329	8.813	21.305	1.00 41.86	0
	MOTA	1069	CG2	THR A 173	-7.666	9.370	21.133	1.00 42.41	С
	MOTA	1070	С	THR A 173	-4.667	11.738	21.003	1.00 40.29	С
	MOTA	1071	0	THR A 173	-3.575	11.623	20.446	1.00 39.42	0
10	MOTA	1072	N	GLU A 174	-4.853	12.487	22.085	1.00 41.07	N
	MOTA	1073	CA	GLU A 174	-3.757	13.227	22.690	1.00 41.95	С
	MOTA	1074	СВ	GLU A 174	-4.264	14.047	23.877	1.00 42.62	С
	MOTA	1075	CG	GLU A 174	-5.227	15.138	23.465	1.00 46.48	С
	MOTA	1076	·CD	GLU A 174	-5.351	16.234	24.497	1.00 52.49	С
15	MOTA	1077	OE1	GLU A 174	-5.735	15.926	25.647	1.00 55.08	0
	MOTA	1078	OE2	GLU A 174	-5.063	17.404	24.154	1.00 53.65	0
	MOTA	1079	С	GLU A 174	-2.621	12.311	23.128	1.00 41.47	С
	MOTA	1080	0	GLU A 174	-1.451	12.688	23.063	1.00 41.74	0
	MOTA	1081	N	GLU A 175	-2.964	11.107	23.569	1.00 40.71	N
20	MOTA	1082	CA	GLU A 175	-1.950	10.149	23.985	1.00 41.13	С
	MOTA	1083	CB	GLU A 175	-2.612	8.908	24.580	1.00 41.37	С
	MOTA	1084	CG	GLU A 175	-3.614	8.278	23.631	1.00 47.30	С
	MOTA	1085	CD	GLU A 175	-4.310	7.065	24.212	1.00 54.26	С
	MOTA	1086	OE1	GLU A 175	-4.885	7.182	25.316	1.00 55.90	0
25	ATOM	1087	OE2	GLU A 175	-4.287	5.998	23.556	1.00 56.76	0

	MOTA	1088	С	GLU A 17	5 -1.12	7 9.760	22.759	1.00 39.75	С
	MOTA	1089	0	GLU A 17	5 -0.00	8 9.256	22.878	1.00 40.30	0
	MOTA	1090	N	ASP A 17	6 -1.68	8 9.995	21.578	1.00 37.64	N
	ATOM	1091	CA	ASP A 17	6 -1.00	9.678	20.328	1.00 36.84	С
5	MOTA	1092	СВ	ASP A 17	6 -1.99	4 9.192	19.265	1.00 37.43	С
	ATOM	1093	CG	ASP A 17	6 -2.51	0 7.795	19.532	1.00 39.43	С
	ATOM	1094	OD1	ASP A 17	6 -1.68	0 6.870	19.681	1.00 42.70	0
	ATOM	1095	OD2	ASP A 17	6 -3.74	6 7.621	19.577	1.00 40.96	0
	MOTA	1096	С	ASP A 17	6 -0.24	7 10.884	19.767	1.00 34.37	С
10	MOTA	1097	0	ASP A 17	6 0.384	10.787	18.723	1.00 33.91	0
	MOTA	1098	N	ILE A 17	7 -0.31	4 12.010	20.466	1.00 32.64	N
	ATOM	1099	CA	ILE A 17	7 0.340	13.237	20.020	1.00 30.44	С
	MOTA	1100	СВ	ILE A 17	7 -0.68	2 14.392	19.970	1.00 30.45	С
	ATOM	1101	CG1	ILE A 17	7 -1.81	2 14.034	18.994	1.00 29.49	С
15	ATOM	1102	CD1	ILE A 17	7 -3.02	9 14.940	19.082	1.00 31.49	С
	MOTA	1103	CG2	ILE A 17	7 0.008	15.688	19.568	1.00 29.62	С
	ATOM	1104	С	ILE A 17	7 1.499	13.633	20.933	1.00 29.89	С
	MOTA	1105	0	ILE A 17	7 1.359	13.647	22.154	1.00 28.34	0
	MOTA	1106	N	VAL A 17	8 2.645	13.960	20.342	1.00 28.91	N
20	MOTA	1107	CA	VAL A 17	8 3.803	14.337	21.142	1.00 28.66	С
	MOTA	1108	СВ	VAL A 17	8 4.711	13.111	21.412	1.00 28.61	С
	MOTA	1109	CG1	VAL A 17	8 5.249	12.566	20.101	1.00 30.80	С
	MOTA	1110	CG2	VAL A 17	8 5.862	13.501	22.331	1.00 30.83	С
	MOTA	1111	С	VAL A 17	8 4.663	15.430	20.522	1.00 27.43	С
25	MOTA	1112	0	VAL A 17	8 4.968	15.402	19.332	1.00 26.89	0

	MOTA	1113	N	PHE A	179	5.043	16.402	21.339	1.00 27.15	N
	ATOM	1114	CA	PHE A	179	5.905	17.478	20.881	1.00 27.17	С
	ATOM	1115	СВ	PHE A	179	5.451	18.813	21.477	1.00 26.48	С
	ATOM	1116	CG	PHE A	179	4.115	19.257	20.961	1.00 27.02	С
5	ATOM	1117	CD1	PHE A	179	3.979	19.704	19.650	1.00 26.14	С
	ATOM	1118	CE1	PHE A	179	2.724	20.041	19.136	1.00 28.69	С
	ATOM	1119	CZ	PHE A	179	1.593	19.930	19.939	1.00 27.93	С
	ATOM	1120	CE2	PHE A	179	1.717	19.488	21.250	1.00 27.21	С
	ATOM	1121	CD2	PHE A	179	2.974	19.156	21.755	1.00 30.11	С
10	ATOM	1122	С	PHE A	179	7.306	17.088	21.323	1.00 27.37	С
	ATOM	1123	0	PHE A	179	7.644	17.138	22.509	1.00 27.77	0
	ATOM	1124	N	LEU A	180	8.093	16.665	20.337	1.00 27.22	N
	ATOM	1125	CA	LEU A	180	9.458	16.194	20.513	1.00 26.96	С
	ATOM	1126	CB	LEU A	180	10.075	15.921	19.134	1.00 26.82	С
15	ATOM	1127	CG	LEU A	180	9.260	14.959	18.257	1.00 26.68	С
	ATOM	1128	CD1	LEU A	180	9.924	14.776	16.901	1.00 21.86	С
•	ATOM	1129	CD2	LEU A	180	9.123	13.616	18.966	1.00 21.60	С
	ATOM	1130	С	LEU A	180	10.362	17.113	21.332	1.00 28.51	С
	ATOM	1131	0	LEU A	180	10.543	18.288	21.004	1.00 28.44	0
20	ATOM	1132	N	PRO A	181	10.943	16.579	22.421	1.00 29.38	N
	ATOM	1133	CA	PRO A	181	11.826	17.378	23.271	1.00 30.92	С
	ATOM	1134	СВ	PRO A	181	11.957	16.524	24.528	1.00 30.61	С
	ATOM	1135	CG	PRO A	181	11.939	15.148	23.982	1.00 29.83	С
	ATOM	1136	CD	PRO A	181	10.827	15.204	22.940	1.00 29.63	С
25	MOTA	1137	С	PRO A	181	13.164	17.622	22.590	1.00 31.85	С

	MOTA	1138	0	PRO A	181	13.683	16.764	21.875	1.00	32.03	0
	MOTA	1139	N	GLN A	182	13.700	18.814	22.812	1.00	34.15	N
	ATOM	1140	CA	GLN A	182	14.972	19.230	22.248	1.00	38.42	С
	MOTA	1141	СВ	GLN A	182	15.160	20.727	22.513	1.00	38.11	С
5	ATOM	1142	CG	GLN A	182	16.349	21.358	21.838	1.00	43.04	С
	ATOM	1143	CD	GLN A	182	16.516	22.813	22.231	1.00	47.27	С
	ATOM	1144	OE1	GLN A	182	15.580	23.609	22.117	1.00	48.82	0
	ATOM	1145	NE2	GLN A	182	17.711	23.170	22.697	1.00	49.54	N
	MOTA	1146	С	GLN A	182	16.112	18.428	22.879	1.00	39.16	С
10	ATOM	1147	0	GLN A	182	16.316	18.480	24.086	1.00	38.96	0
	ATOM	1148	N	PRO A	183	16.859	17.662	22.064	1.00	41.26	N
	ATOM	1149	CA	PRO A	183	17.982	16.847	22.544	1.00	43.14	С
	MOTA	1150	СВ	PRO A	183	18.400	16.062	21.301	1.00	42.53	С
	MOTA	1151	CG	PRO A	183	17.158	16.009	20.489	1.00	42.51	С
15	ATOM	1152	CD	PRO A	183	16.605	17.398	20.641	1.00	41.37	С
	ATOM	1153	С	PRO A	183	19.108	17.739	23.043	1.00	45.17	С
	MOTA	1154	0	PRO A	183	19.222	18.894	22.630	1.00	45.74	0
	ATOM	1155	N	ASP A	184	19.939	17.208	23.931	1.00	47.82	N
	MOTA	1156	CA	ASP A	184	21.059	17.974	24.468	1.00	50.56	С
20	ATOM	1157	СВ	ASP A	184	21.516	17.365	25.799	1.00	51.23	С
	ATOM	1158	CG	ASP A	184	22.507	18.246	26.543	1.00	54.35	С
	MOTA	1159	OD1	ASP A	184	23.479	18.717	25.914	1.00	58.16	0
	MOTA	1160	OD2	ASP A	184	22.324	18.461	27.763	1.00	57.05	0
	MOTA	1161	С	ASP A	184	22.203	17.949	23.453	1.00	51.40	С
25	MOTA	1162	0	ASP A	184	22.988	18.890	23.366	1.00	52.48	0

	MOTA	1163	N	LYS A 185	22.284	16.869	22.684	1.00 52.40	N
	ATOM	1164	CA	LYS A 185	23.319	16.719	21.668	1.00 53.25	С
	MOTA	1165	СВ	LYS A 185	24.352	15.684	22.118	1.00 53.85	С
	ATOM	1166	CG	LYS A 185	23.763	14.312	22.430	1.00 54.84	С
5	ATOM	1167	CD	LYS A 185	24.851	13.323	22.816	1.00 57.25	С
	ATOM	1168	CE	LYS A 185	24.267	11.984	23.237	1.00 59.39	С
	ATOM	1169	NZ	LYS A 185	25.336	11.017	23.617	1.00 59.87	N
	ATOM	1170	С	LYS A 185	22.716	16.284	20.334	1.00 53.50	С
	ATOM	1171	0	LYS A 185	21.499	16.182	20.199	1.00 53.06	0
10	ATOM	1172	N	CYS A 186	23.585	16.034	19.357	1.00 54.14	N
	ATOM	1173	CA	CYS A 186	23.183	15.596	18.021	1.00 55.37	С
	ATOM	1174	СВ	CYS A 186	22.282	14.353	18.107	1.00 54.41	С
	ATOM	1175	SG	CYS A 186	22.903	12.974	19.126	1.00 51.22	S
	ATOM	1176	С	CYS A 186	22.467	16.652	17.176	1.00 56.92	С
15	ATOM	1177	0	CYS A 186	21.884	16.315	16.147	1.00 57.78	0
	ATOM	1178	N	ILE A 187	22.513	17.919	17.580	1.00 59.30	N
	MOTA	1179	CA	ILE A 187	21.817	18.953	16.812	1.00 61.99	С
	ATOM	1180	СВ	ILE A 187	20.357	19.109	17.314	1.00 62.28	С
	ATOM	1181	CG1	ILE A 187	19.545	17.872	16.927	1.00 61.77	С
20	ATOM	1182	CD1	ILE A 187	18.090	17.965	17.308	1.00 65.79	С
	MOTA	1183	CG2	ILE A 187	19.710	20.354	16.726	1.00 63.84	С
	MOTA	1184	С	ILE A 187	22.440	20.346	16.751	1.00 63.97	С
	MOTA	1185	0	ILE A 187	22.046	21.143	15.904	1.00 64.66	0
	MOTA	1186	N	GLN A 188	23.412	20.642	17.609	1.00 66.08	N
25	MOTA	1187	CA	GLN A 188	24.019	21.978	17.637	1.00 68.34	С

	MOTA	1188	СВ	GLN A	A 188	24.150	22.572	16.226	1.00 68.29	С
	MOTA	1189	CG	GLN A	A 188	25.566	22.753	15.711	1.00 70.61	С
	MOTA	1190	CD	GLN A	A 188	26.306	21.441	15.570	1.00 72.82	С
	MOTA	1191	OE1	GLN A	A 188	25.787	20.479	14.999	1.00 73.93	0
5	MOTA	1192	NE2	GLN A	A 188	27.531	21.395	16.082	1.00 74.08	N
	MOTA	1193	С	GLN A	A 188	23.042	22.830	18.444	1.00 69.30	С
	MOTA	1194	0	GLN A	A 188	23.017	24.055	18.331	1.00 69.66	0
	MOTA	1195	N	GLU A	A 189	22.232	22.135	19.242	1.00 70.42	N
	MOTA	1196	CA	GLU A	A 189	21.203	22.703	20.112	1.00 71.39	С
10	MOTA	1197	СВ	GLU A	A 189	21.351	22.125	21.520	1.00 71.77	С
	MOTA	1198	CG	GLU A	A 189	22.147	20.827	21.579	1.00 72.99	С
	MOTA	1199	CD	GLU A	A 189	21.669	19.790	20.583	1.00 73.77	С
	MOTA	1200	OE1	GLU A	A 189	20.472	19.433	20.610	1.00 76.28	0
	MOTA	1201	OE2	GLU A	A 189	22.494	19.324	19.770	1.00 73.47	0
15	MOTA	1202	С	GLU A	A 189	21.165	24.227	20.195	1.00 71.75	С
	MOTA	1203	0	GLU A	A 189	21.377	24.768	21.303	1.00 71.94	0
	MOTA	1204	OXT	GLU A	A 189	20.906	24.868	19.153	1.00 72.13	0
	MOTA	1205	N	GLN I	35	16.520	25.594	58.782	1.00 37.06	N
	MOTA	1206	CA	GLN I	3 35	16.131	26.126	57.446	1.00 35.29	С
20	MOTA	1207	СВ	GLN I	35	17.377	26.612	56.704	1.00 35.86	С
	MOTA	1208	CG	GLN I	35	18.466	25.564	56.576	1.00 40.43	С
	MOTA	1209	CD	GLN I	35	19.622	26.021	55.700	1.00 46.53	С
	MOTA	1210	OE1	GLN I	35	20.623	25.313	55.554	1.00 51.77	0
	MOTA	1211	NE2	GLN I	в 35	19.487	27.204	55.107	1.00 49.87	N
25	ATOM	1212	С	GLN I	в 35	15.384	25.108	56.577	1.00 33.30	С

	MOTA	1213	0	GLN B	35	15.044	25.406	55.435	1.00 32.10	0
	MOTA	1214	N	GLN B	36	15.123	23.917	57.113	1.00 31.25	N
	MOTA	1215	CA	GLN B	36	14.423	22.876	56.353	1.00 29.23	С
	MOTA	1216	СВ	GLN B	36	14.196	21.618	57.203	1.00 29.22	С
5	MOTA	1217	CG	GLN B	36	13.615	20.451	56.401	1.00 30.50	С
	MOTA	1218	CD	GLN B	36	13.423	19.185	57.222	1.00 31.43	С
	MOTA	1219	OE1	GLN B	36	12.508	19.086	58.053	1.00 36.00	0
	MOTA	1220	NE2	GLN B	36	14.290	18.209	56.996	1.00 27.78	N
	MOTA	1221	С	GLN B	36	13.083	23.366	55.840	1.00 26.86	С
10	MOTA	1222	0	GLN B	36	12.708	23.095	54.699	1.00 23.30	0
	MOTA	1223	N	ASP B	37	12.363	24.084	56.694	1.00 27.22	N
	MOTA	1224	CA	ASP B	37	11.050	24.609	56.338	1.00 27.10	С
	MOTA	1225	СВ	ASP B	37	10.457	25.408	57.499	1.00 30.98	С
	MOTA	1226	CG	ASP B	37	9.837	24.522	58.561	1.00 35.24	С
15	MOTA	1227	OD1	ASP B	37	10.576	23.732	59.182	1.00 47.18	0
	MOTA	1228	OD2	ASP B	37	8.609	24.616	58.778	1.00 45.07	0
	MOTA	1229	С	ASP B	37	11.066	25.480	55.097	1.00 25.31	С
	MOTA ·	1230	0	ASP B	37	10.045	25.635	54.435	1.00 24.94	0
	MOTA	1231	N	LYS B	38	12.223	26.054	54.786	1.00 24.03	Ŋ
20	MOTA	1232	CA	LYS B	38	12.345	26.911	53.617	1.00 23.34	С
	MOTA	1233	СВ	LYS B	38	13.643	27.722	53.691	1.00 23.59	С
	MOTA	1234	CG	LYS B	38	13.641	28.770	54.800	1.00 26.63	С
	MOTA	1235	CD	LYS B	38	12.474	29.733	54.619	1.00 28.10	С
	MOTA	1236	CE	LYS B	38	12.507	30.861	55.636	1.00 34.26	С
25	MOTA	1237	NZ	LYS B	38	13.727	31.698	55.494	1.00 36.28	N

	MOTA	1238	С	LYS B	38	12.297	26.139	52.304	1.00 22.17	С
	MOTA	1239	0	LYS B	38	12.019	26.719	51.262	1.00 23.22	.0
	MOTA	1240	N	PHE B	39	12.555	24.836	52.362	1.00 19.91	N
	MOTA	1241	CA	PHE B	39	12.561	24.000	51.171	1.00 17.90	С
5	MOTA	1242	СВ	PHE B	39	13.749	23.033	51.226	1.00 19.08	С
	MOTA	1243	CG	PHE B	39	15.089	23.725	51.228	1.00 18.43	С
	MOTA	1244	CD1	PHE B	39	15.607	24.265	52.398	1.00 16.91	С
	MOTA	1245	CE1	PHE B	39	16.823	24.930	52.401	1.00 19.03	С
	MOTA	1246	CZ	PHE B	39	17.546	25.067	51.211	1.00 20.75	С
10	MOTA	1247	CE2	PHE B	39	17.035	24.531	50.034	1.00 21.98	С
	MOTA	1248	CD2	PHE B	39	15.811	23.862	50.050	1.00 19.07	С
	MOTA	1249	С	PHE B	39	11.270	23.224	50.967	1.00 16.73	С
	MOTA	1250	0	PHE B	39	11.175	22.390	50.068	1.00 16.56	0
	MOTA	1251	N	LEU B	40	10.272	23.492	51.800	1.00 15.91	N
15	MOTA	1252	CA	LEU B	40	9.000	22.803	51.653	1.00 17.17	С
	MOTA	1253	СВ	LEU B	40	8.113	23.043	52.878	1.00 17.42	С
	MOTA	1254	CG	LEU B	40	8.753	22.577	54.192	1.00 19.17	С
	MOTA	1255	CD1	LEU B	40	7.779	22.756	55.337	1.00 24.49	С
	MOTA	1256	CD2	LEU B	40	9.161	21.117	54.075	1.00 20.54	С
20	MOTA	1257	С	LEU B	40	8.345	23.357	50.401	1.00 17.51	С
	MOTA	1258	0	LEU B	40	8.832	24.325	49.816	1.00 17.99	0
	MOTA	1259	N	GLY B	41	7.266	22.729	49.960	1.00 17.31	N
	MOTA	1260	CA	GLY B	41	6.588	23.237	48.783	1.00 17.09	С
	MOTA	1261	С	GLY B	41	6.856	22.523	47.477	1.00 17.14	С
25	MOTA	1262	0	GLY B	41	7.352	21.394	47.444	1.00 18.05	0

	MOTA	1263	N	ARG B	42	6.543	23.215	46.389	1.00 16.40	N
	ATOM	1264	CA	ARG B	42	6.680	22.676	45.043	1.00 18.88	С
	ATOM	1265	СВ	ARG B	42	5.614	23.311	44.155	1.00 17.27	С
	ATOM	1266	CG	ARG B	42	5.756	22.949	42.697	1.00 25.31	С
5	ATOM	1267	CD	ARG B	42	5.545	24.170	41.836	1.00 28.18	С
	ATOM	1268	NE	ARG B	42	4.160	24.356	41.464	1.00 27.84	N
	ATOM	1269	CZ	ARG B	42	3.700	25.456	40.879	1.00 32.90	C
	ATOM	1270	NH1	ARG B	42	4.526	26.466	40.622	1.00 29.84	N
	MOTA	1271	NH2	ARG B	42	2.428	25.527	40.509	1.00 28.11	N
10	ATOM	1272	С	ARG B	42	8.043	22.809	44.355	1.00 17.36	С
	ATOM	1273	0	ARG B	42	8.626	23.894	44.278	1.00 16.56	0
	MOTA	1274	N	TRP B	43	8.530	21.686	43.837	1.00 18.23	N
	ATOM	1275	CA	TRP B	43	9.796	21.653	43.113	1.00 17.56	С
	ATOM	1276	CB	TRP B	43	10.903	21.021	43.949	1.00 16.97	С
15	ATOM	1277	CG	TRP B	43	11.305	21.771	45.176	1.00 16.19	С
	ATOM	1278	CD1	TRP B	43	10.757	21.668	46.424	1.00 17.38	С
	ATOM	1279	NE1	TRP B	43	11.444	22.462	47.312	1.00 14.16	N
	ATOM	1280	CE2	TRP B	43	12.452	23.102	46.641	1.00 14.82	С
	ATOM	1281	CD2	TRP B	43	12.393	22.692	45.290	1.00 15.35	С
20	ATOM	1282	CE3	TRP B	43	13.322	23.210	44.384	1.00 13.96	С
	ATOM	1283	CZ3	TRP B	43	14.281	24.114	44.850	1.00 18.19	С
	ATOM	1284	CH2	TRP B	43	14.313	24.501	46.202	1.00 16.46	С
	ATOM	1285	CZ2	TRP B	43	13.409	24.008	47.107	1.00 16.31	С
	MOTA	1286	С	TRP B	43	9.621	20.813	41.863	1.00 17.89	С
25	MOTA	1287	0	TRP B	43	8.650	20.071	41.733	1.00 17.99	0

	MOTA	1288	N	TYR B	44	10.579	20.925	40.952	1.00 18.35	N
	MOTA	1289	CA	TYR B	44	10.568	20.162	39.712	1.00 19.01	С
	MOTA	1290	СВ	TYR B	44	10.294	21.085	38.523	1.00 20.26	C
	MOTA	1291	CG	TYR B	44	8.927	21.731	38.531	1.00 19.50	С
5	MOTA	1292	CD1	TYR B	44	7.799	21.020	38.120	1.00 21.39	С
	MOTA	1293	CE1	TYR B	44	6.529	21.605	38.129	1.00 21.89	С
	MOTA	1294	CZ	TYR B	44	6.387	22.916	38.557	1.00 23.64	С
	MOTA	1295	OH	TYR B	44	5.135	23.485	38.590	1.00 21.63	0
	MOTA	1296	CE2	TYR B	44	7.496	23.647	38.973	1.00 22.08	С
10	MOTA	1297	CD2	TYR B	44	8.760	23:050	38.958	1.00 21.31	С
	MOTA	1298	С	TYR B	44	11.937	19.506	39.528	1.00 20.14	С
	MOTA	1299	0	TYR B	44	12.979	20.175	39.631	1.00 19.15	0
	MOTA	1300	N	SER B	45	11.940	18.197	39.273	1.00 21.35	N
	MOTA	1301	CA	SER B	45	13.192	17.487	39.032	1.00 23.58	С
15	MOTA	1302	СВ	SER B	45	12.987	15.970	39.141	1.00 25.18	С
	MOTA	1303	OG	SER B	45	11.926	15.531	38.307	1.00 26.39	0
	MOTA	1304	С	SER B	45	13.585	17.878	37.612	1.00 24.18	С
	MOTA	1305	0	SER B	45	12.903	17.521	36.656	1.00 25.49	0
	MOTA	1306	N	ALA B	46	14.680	18.627	37.484	1.00 24.22	N
20	MOTA	1307	CA	ALA B	46	15.136	19.102	36.186	1.00 21.23	С
	MOTA	1308	СВ	ALA B	46	15.312	20.621	36.231	1.00 20.41	С
	MOTA	1309	С	ALA B	46	16.423	18.458	35.693	1.00 21.73	С
	ATOM	1310	0	ALA B	46	16.724	18.505	34.503	1.00 21.13	0
	ATOM	1311	N	GLY B	47	17.195	17.878	36.605	1.00 22.14	N
25	ATOM	1312	CA	GLY B	47	18.452	17.261	36.217	1.00 22.69	С

	MOTA	1313	С	GLY B	47	18.706	15.987	36.987	1.00 22.41	С
	MOTA	1314	0	GLY B	47	18.440	15.922	38.186	1.00 21.93	0
	MOTA	1315	N	LEU B	48	19.219	14.973	36.296	1.00 24.68	N
	MOTA	1316	CA	LEU B	48	19.496	13.682	36.919	1.00 26.44	С
5	MOTA	1317	СВ	LEU B	48	18.288	12.762	36.740	1.00 25.78	С
	MOTA	1318	CG	LEU B	48	18.301	11.366	37.357	1.00 27.38	С
	MOTA	1319	CD1	LEU B	48	18.364	11.455	38.880	1.00 31.44	С
	MOTA	1320	CD2	LEU B	48	17.031	10.633	36.942	1.00 29.28	С
	MOTA	1321	С	LEU B	48	20.744	13.035	36.315	1.00 28.13	С
10	MOTA	1322	0	LEU B	48	20.924	13.018	35.096	1.00 28.67	0
	MOTA	1323	N	ALA B	49	21.608	12.513	37.177	1.00 29.37	N
	MOTA	1324	CA	ALA B	49	22.836	11.860	36.736	1.00 30.98	С
	MOTA	1325	СВ	ALA B	49	23.987	12.849	36.763	1.00 29.77	С
	MOTA	1326	С	ALA B	49	23.134	10.674	37.650	1.00 32.18	С
15	MOTA	1327	0	ALA B	49	22.876	10.731	38.849	1.00 32.22	0
	MOTA	1328	N	SER B	50	23.671	9.598	37.084	1.00 34.77	N
	MOTA	1329	CA	SER B	50	23.980	8.408	37.872	1.00 36.25	С
•	MOTA	1330	СВ	SER B	50	22.684	7.746	38.339	1.00 35.93	С
	MOTA	1331	OG	SER B	50	22.950	6.569	39.084	1.00 36.08	0
20	MOTA	1332	С	SER B	50	24.815	7.386	37.109	1.00 37.63	С
	MOTA	1333	0	SER B	50	25.029	7.518	35.903	1.00 38.29	0
	MOTA	1334	N	ASN B	51	25.287	6.369	37.825	1.00 38.85	N
	MOTA	1335	CA	ASN B	51	26.076	5.302	37.222	1.00 40.59	С
	MOTA	1336	СВ	ASN B	51	27.459	5.203	37.880	1.00 40.57	С
25	ATOM	1337	CG	ASN B	51	27.391	4.940	39.380	1.00 39.49	С

	MOTA	1338	OD1	ASN B	51	28.419	4.773	40.030	1.00 42.49	0
	MOTA	1339	ND2	ASN B	51	26.185	4.903	39.931	1.00 34.80	N
	MOTA	1340	С	ASN B	51	25.328	3.984	37.377	1.00 42.31	С
	MOTA	1341	0	ASN B	51	25.792	2.935	36.941	1.00 42.26	0
5	MOTA	1342	N	SER B	52	24.160	4.058	38.004	1.00 44.68	N
	MOTA	1343	CA	SER B	52	23.323	2.888	38.233	1.00 47.48	С
	MOTA	1344	СВ	SER B	52	22.033	3.306	38.944	1.00 48.00	С
	MOTA	1345	OG	SER B	52	21.065	2.269	38.892	1.00 52.56	0
	MOTA	1346	С	SER B	52	22.964	2.146	36.952	1.00 48.12	С
10	MOTA	1347	0	SER B	52	23.280	2.590	35.850	1.00 48.41	0
	MOTA	1348	N	SER B	53	22.301	1.006	37.118	1.00 49.66	N
	MOTA	1349	CA	SER B	53	21.859	0.188	35.996	1.00 50.25	С
	MOTA	1350	СВ	SER B	53	21.713	-1.273	36.437	1.00 50.27	С
	MOTA	1351	OG	SER B	53	22.947	-1.793	36.907	1.00 51.05	0
15	MOTA	1352	С	SER B	53	20.507	0.745	35.567	1.00 50.62	С
	MOTA	1353	0	SER B	53	20.218	0.874	34.378	1.00 50.70	O
	MOTA	1354	N	TRP B	54	19.693	1.077	36.564	1.00 51.37	N
	MOTA	1355	CA	TRP B	54	18.364	1.638	36.358	1.00 52.70	С
	MOTA	1356	СВ	TRP B	54	17.776	2.047	37.709	1.00 53.23	С
20	MOTA	1357	CG	TRP B	54	16.450	2.737	37.630	1.00 56.64	С
	MOTA	1358	CD1	TRP B	54	15.234	2.162	37.391	1.00 59.22	С
	MOTA	1359	NE1	TRP B	54	14.244	3.119	37.411	1.00 60.28	N
	MOTA	1360	CE2	TRP B	54	14.813	4.340	37.661	1.00 60.04	С
	MOTA	1361	CD2	TRP B	54	16.205	4.138	37.804	1.00 58.84	С
25	MOTA	1362	CE3	TRP B	54	17.027	5.243	38.068	1.00 59.81	С

	MOTA	1363	CZ3	TRP B	54	16.441	6.500	38.179	1.00 60.48	C
	ATOM	1364	CH2	TRP B	54	15.052	6.669	38.032	1.00 61.73	С
	ATOM	1365	CZ2	TRP B	54	14.224	5.606	37.774	1.00 61.41	С
	ATOM	1366	С	TRP B	54	18.439	2.855	35.441	1.00 52.10	С
5	ATOM	1367	0	TRP B	54	17.820	2.889	34.373	1.00 52.71	0
	ATOM	1368	N	PHE B	55	19.205	3.851	35.869	1.00 51.33	N
	ATOM	1369	CA	PHE B	55	19.376	5.082	35.109	1.00 50.85	С
	ATOM	1370	СВ	PHE B	55	20.395	5.984	35.812	1.00 50.43	С
	ATOM	1371	CG	PHE B	55	20.594	7.314	35.146	1.00 48.28	С
10	ATOM	1372	CD1	PHE B	55	19.562	8.245	35.099	1.00 46.15	С
	ATOM	1373	CE1	PHE B	55	19.740	9.474	34.471	1.00 46.51	С
	ATOM	1374	CZ	PHE B	55	20.960	9.780	33.881	1.00 46.07	С
	ATOM	1375	CE2	PHE B	55	21.998	8.856	33.923	1.00 46.09	С
	ATOM	1376	CD2	PHE B	55	21.810	7.632	34.553	1.00 46.98	С
15	ATOM	1377	С	PHE B	55	19.826	4.801	33.677	1.00 51.09	С
	ATOM	1378	0	PHE B	55	19.209	5.271	32.719	1.00 51.00	0
	ATOM	1379	N	ARG B	56	20.903	4.034	33.541	1.00 51.57	N
	ATOM	1380	CA	ARG B	56	21.445	3.677	32.229	1.00 52.15	С
	ATOM	1381	СВ	ARG B	56	22.640	2.726	32.393	1.00 52.46	С
20	MOTA	1382	CG	ARG B	56	23.954	3.386	32.783	1.00 54.53	С
	MOTA	1383	CD	ARG B	56	24.907	2.357	33.397	1.00 58.48	С
	MOTA	1384	NE	ARG B	56	26.299	2.806	33.475	1.00 62.11	N
	MOTA	1385	CZ	ARG B	56	26.693	3.976	33.970	1.00 65.15	С
	MOTA	1386	NH1	ARG B	56	25.802	4.841	34.437	1.00 66.66	N
25	MOTA	1387	NH2	ARG B	56	27.984	4.281	34.006	1.00 65.67	N

	MOTA	1388	С	ARG B	56	20.411	3.027	31.306	1.00 51.62	С
	MOTA	1389	0	ARG B	56	20.424	3.258	30.099	1.00 51.26	0
	MOTA	1390	N	GLU B	57	19.515	2.223	31.872	1.00 51.11	N
	MOTA	1391	CA	GLU B	57	18.507	1.540	31.071	1.00 51.51	С
5	MOTA	1392	СВ	GLU B	57	18.503	0.046	31.415	1.00 51.87	С
	MOTA	1393	CG	GLU B	57	19.780	-0.677	31.007	1.00 53.93	С
	MOTA	1394	CD	GLU B	57	19.773	-2.151	31.375	1.00 56.43	С
	MOTA	1395	OE1	GLU B	57	19.748	-2.462	32.585	1.00 58.93	0
•	MOTA	1396	OE2	GLU B	57	19.794	-2.996	30.452	1.00 56.91	0
10	MOTA	1397	С	GLU B	57	17.094	2.107	31.210	1.00 50.67	С
	MOTA	1398	0	GLU B	57	16.108	1.381	31.058	1.00 51.18	0
	ATOM	1399	N	LYS B	58	16.991	3.402	31.491	1.00 49.06	N
	MOTA	1400	CA	LYS B	58	15.683	4.039	31.646	1.00 47.54	C
	MOTA	1401	CB	LYS B	58	15.107	3.722	33.032	1.00 48.39	С
15	MOTA	1402	CG	LYS B	58	13.686	4.226	33.258	1.00 49.62	С
	MOTA	1403	CD	LYS B	58	13.212	3.952	34.682	1.00 52.77	С
	ATOM	1404	CE	LYS B	58	11.825	4.545	34.941	1.00 52.82	С
	MOTA	1405	NZ	LYS B	58	11.389	4.377	36.358	1.00 52.01	N
	MOTA	1406	С	LYS B	58	15.764	5.549	31.457	1.00 45.21	С
20	MOTA	1407	0	LYS B	58	14.746	6.226	31.389	1.00 44.48	0
	MOTA	1408	N	LYS B	59	16.983	6.065	31.359	1.00 43.69	N
	MOTA	1409	CA	LYS B	59	17.211	7.494	31.189	1.00 42.38	С
	MOTA	1410	СВ	LYS B	59	18.709	7.758	31.034	1.00 43.61	С
	MOTA	1411	CG	LYS B	59	19.336	7.073	29.832	1.00 44.44	С
25	MOTA	1412	CD	LYS B	59	20.858	7.044	29.928	1.00 49.79	С

	MOTA	1413	CE	LYS B	59	21.441	8.431	30.163	1.00 52.89	С
	MOTA	1414	NZ	LYS B	59	21.020	9.404	29.118	1.00 56.53	N
	MOTA	1415	С	LYS B	59	16.459	8.087	30.003	1.00 40.91	С
	MOTA	1416	0	LYS B	59	15.966	9.213	30.071	1.00 40.09	0
5	MOTA	1417	N	ALA B	60	16.367	7.324	28.919	1.00 39.16	N
	MOTA	1418	CA	ALA B	60	15.682	7.785	27.723	1.00 36.81	С
	MOTA	1419	СВ	ALA B	60	15.850	6.773	26.605	1.00 37.20	С
	MOTA	1420	С	ALA B	60	14.200	8.054	27.952	1.00 35.75	С
	MOTA	1421	0	ALA B	60	13.627	8.923	27.300	1.00 35.18	0
10	MOTA	1422	N	VAL B	61	13.584	7.319	28.875	1.00 33.10	N
	MOTA	1423	CA	VAL B	61	12.157	7.485	29.147	1.00 32.61	С
	MOTA	1424	СВ	VAL B	61	11.462	6.114	29.347	1.00 32.54	С
	MOTA	1425	CG1	VAL B	61	11.692	5.234	28.127	1.00 33.11	С
	MOTA	1426	CG2	VAL B	61	11.981	5.434	30.612	1.00 31.73	С
15	MOTA	1427	С	VAL B	61	11.832	8.353	30.358	1.00 31.55	С
	MOTA	1428	0	VAL B	61	10.675	8.446	30.761	1.00 31.40	0
	MOTA	1429	N	LEU B	62	12.844	8:991	30.935	1.00 30.56	N
	MOTA	1430	CA	LEU B	62	12.621	9.839	32.103	1.00 30.36	С
	MOTA	1431	СВ	LEU B	62	13.877	9.865	32.975	1.00 31.00	С
20	MOTA	1432	CG	LEU B	62	14.292	8.491	33.516	1.00 33.97	С
	MOTA	1433	CD1	LEU B	62	15.598	8.599	34.288	1.00 33.22	C.
	MOTA	1434	CD2	LEU B	62	13.183	7.942	34.407	1.00 34.87	С
	MOTA	1435	С	LEU B	62	12.212	11.265	31.740	1.00 27.77	С
	ATOM	1436	0	LEU B	62	12.790	11.881	30.849	1.00 27.70	0
25	ATOM	1437	N	TYR B	63	11.196	11.772	32.431	1.00 27.50	N

	MOTA	1438	CA	TYR B	63	10.705	13.127	32.211	1.00 26.18	С
	ATOM	1439	СВ	TYR B	63	9.240	13.133	31.747	1.00 26.26	С
	MOTA	1440	CG	TYR B	63	8.992	12.606	30.357	1.00 27.42	С
	MOTA	1441	CD1	TYR B	63	8.814	11.243	30.127	1.00 29.98	С
5	MOTA	1442	CE1	TYR B	63	8.572	10.757	28.843	1.00 33.87	С
	ATOM	1443	CZ	TYR B	63	8.514	11.640	27.775	1.00 32.87	С
	ATOM	1444	OH	TYR B	63	8.286	11.168	26.500	1.00 38.94	0
	ATOM	1445	CE2	TYR B	63	8.691	13.000	27.981	1.00 32.51	С
	ATOM	1446	CD2	TYR B	63	8.926	13.474	29.268	1.00 28.18	С
10	MOTA	1447	С	TYR B	63	10.783	13.909	33.513	1.00 24.64	С
	MOTA	1448	0	TYR B	63	10.958	13.335	34.580	1.00 26.37	0
	ATOM	1449	N	MET B	64	10.654	15.224	33.406	1.00 24.11	N
	ATOM	1450	CA	MET B	64	10.666	16.089	34.564	1.00 21.60	С
	ATOM	1451	СВ	MET B	64	10.551	17.543	34.137	1.00 21.40	С
15	ATOM	1452	CG	MET B	64	10.203	18.491	35.274	1.00 21.55	С
	MOTA	1453	SD	MET B	64	10.078	20.155	34.653	1.00 23.70	S
	ATOM	1454	CE	MET B	64	11.772	20.441	34.213	1:00 23.94	С
	ATOM	1455	С	MET B	64	9.454	15.723	35.391	1.00 20.89	С
	ATOM	1456	0	MET B	64	8.387	15.462	34.841	1.00 20.65	0
20	MOTA	1457	N	ALA B	65	9.620	15.710	36.709	1.00 21.78	N
	ATOM	1458	CA	ALA B	65	8.529	15.381	37.610	1.00 22.90	С
	MOTA	1459	СВ	ALA B	65	8.873	14.137	38.417	1.00 23.61	С
	MOTA	1460	С	ALA B	65	8.243	16.536	38.550	1.00 22.81	С
	ATOM	1461	0	ALA B	65	9.114	17.356	38.829	1.00 23.08	0
25	MOTA	1462	N	LYS B	66	7.008	16.595	39.026	1.00 24.13	N

	MOTA	1463	CA	LYS B	66	6.592	17.625	39.968	1.00 24.90	С
	MOTA	1464	СВ	LYS B	66	5.175	18.090	39.635	1.00 24.40	С
	MOTA	1465	CG	LYS B	66	4.531	19.010	40.658	1.00 25.61	С
	MOTA	1466	CD	LYS B	66	3.216	19.555	40.101	1.00 24.44	С
5	MOTA	1467	CE	LYS B	66	2.390	20.253	41.157	1.00 29.98	С
	MOTA	1468	NZ	LYS B	66	1.154	20.853	40.569	1.00 39.00	N
	MOTA	1469	С	LYS B	66	6.641	16.990	41.356	1.00 24.30	С
	ATOM	1470	0	LYS B	66	5.955	15.999	41.616	1.00 26.16	0
	MOTA	1471	N	THR B	67	7.468	17.543	42.234	1.00 21.31	N
10	MOTA	1472	CA	THR B	67	7.608	17.017	43.582	1.00 20.57	С
	ATOM	1473	СВ	THR B	67	9.066	16.619	43.871	1.00 21.25	С
	MOTA	1474	OG1	THR B	67	9.494	15.626	42.934	1.00 21.89	0
	MOTA	1475	CG2	THR B	67	9.190	16.068	45.285	1.00 25.45	С
	ATOM	1476	С	THR B	67	7.186	18.043	44.639	1.00 20.93	С
15	MOTA	1477	0	THR B	67	7.706	19.165	44.676	1.00 19.49	0
	MOTA	1478	N	VAL B	68	6.244	17.655	45.494	1.00 19.26	N
	MOTA	1479	CA	VAL B	68	5.784	18.536	46.556	1.00 18.83	С
	MOTA	1480	СВ	VAL B	68	4.248	18.560	46.641	1.00 18.95	С
	MOTA	1481	CG1	VAL B	68	3.809	19.454	47.803	1.00 21.13	С
20	MOTA	1482	CG2	VAL B	68	3.675	19.070	45.313	1.00 17.89	С
	MOTA	1483	С	VAL B	68	6.382	18.032	47.848	1.00 17.05	С
	MOTA	1484	0	VAL B	68	6.272	16.850	48.180	1.00 18.24	0
	MOTA	1485	N	VAL B	69	7.038	18.938	48.567	1.00 17.22	N
	MOTA	1486	CA	VAL B	69	7.722	18.593	49.807	1.00 15.35	С
25	MOTA	1487	СВ	VAL B	69	9.151	19.150	49.772	1.00 15.47	С

	MOTA	1488	CG1	VAL B	69	9.898	18.773	51.041	1.00 13.26	С
	MOTA	1489	CG2	VAL B	69	9.875	18.625	48.511	1.00 15.70	С
	MOTA	1490	С	VAL B	69	7.027	19.086	51.077	1.00 15.51	С
	MOTA	1491	0	VAL B	69	6.649	20.256	51.182	1.00 16.17	0
5	MOTA	1492	N	ALA B	70	6.863	18.181	52.036	1.00 16.04	N
	MOTA	1493	CA	ALA B	70	6.229	18.511	53.316	1.00 16.88	С
	MOTA	1494	СВ	ALA B	70	4.739	18.155	53.280	1.00 17.76	С
	MOTA	1495	С	ALA B	70	6.937	17.725	54.413	1.00 16.99	С
	ATOM	1496	0	ALA B	70 .	7.651	16.766	54.126	1.00 19.87	0
10	ATOM	1497	N	PRO B	71	6.742	18.110	55.687	1.00 18.18	N
	ATOM	1498	CA	PRO B	71	7.399	17.407	56.796	1.00 17.02	С
	MOTA	1499	СВ	PRO B	71	6.943	18.192	58.024	1.00 18.58	С
	ATOM	1500	CG	PRO B	71	6.643	19.577	57.471	1.00 19.30	С
	ATOM	1501	CD	PRO B	71	5.930	19.236	56.192	1.00 16.39	С
15	ATOM	1502	С	PRO B	71	7.034	15.930	56.905	1.00 18.37	С
	ATOM	1503	0	PRO B	71 -	5.907	15.537	56.594	1.00 15.78	0
	MOTA	1504	N	SER B	72	7.993	15.122	57.353	1.00 18.33	N
	MOTA	1505	CA	SER B	72	7.769	13.699	57.529	1.00 20.27	С
	MOTA	1506	CB	SER B	72	8.978	12.884	57.061	1.00 21.15	С
20	MOTA	1507	Œ	SER B	72	10.036	12.957	57.997	1.00 23.81	0
	MOTA	1508	С	SER B	72	7.535	13.482	59.016	1.00 21.63	С
	ATOM	1509	0	SER B	72	7.788	14.377	59.825	1.00 22.26	0
	MOTA	1510	N	THR B	73	7.058	12.297	59.378	1.00 22.59	N
	MOTA	1511	CA	THR B	73	6.757	12.006	60.779	1.00 23.74	С
25	MOTA	1512	СВ	THR B	73	6.236	10.564	60.952	1.00 22.91	С

	MOTA	1513	OG1	THR B	73	5.172	10.318	60.025	1.00 18.94	0
	MOTA	1514	CG2	THR B	73	5.697	10.368	62.375	1.00 24.56	С
	MOTA	1515	С	THR B	73	7.926	12.201	61.747	1.00 24.50	С
	MOTA	1516	0	THR B	73	7.758	12.806	62.800	1.00 24.98	0
5 .	MOTA	1517	N	GLU B	74	9.101	11.684	61.389	1.00 25.95	N
	MOTA	1518	CA	GLU B	74	10.287	11.785	62.243	1.00 26.06	С
	ATOM	1519	СВ	GLU B	74	11.271	10.657	61.926	1.00 26.86	С
	ATOM	1520	CG	GLU B	74	10.734	9.266	62.197	1.00 29.93	С
	MOTA	1521	CD	GLU B	74	10.240	9.113	63.612	1.00 34.17	С
10	MOTA	1522	OE1	GLU B	74	11.018	9.405	64.549	1.00 38.32	0
	ATOM	1523	OE2	GLU B	74	9.075	8.701	63.790	1.00 39.68	0
	ATOM	1524	С	GLU B	74	11.028	13.105	62.140	1.00 26.53	С
	MOTA	1525	0	GLU B	74	12.075	13.269	62.754	1.00 26.06	0
	ATOM	1526	N	GLY B	75	10.495	14.042	61.365	1.00 26.90	N
15	ATOM	1527	CA	GLY B	75	11.163	15.321	61.217	1.00 26.25	С
	MOTA	1528	С	GLY B	75	11.902	15.432	59.895	1.00 26.38	С
	MOTA	1529	0	GLY B	75	12.521	16.458	59.607	1.00 27.95	O
	MOTA	1530	N	GLY B	76	11.854	14.367	59.097	1.00 24.68	N
	ATOM	1531	CA	GLY B	76	12.498	14.376	57.796	1.00 22.08	С
20	MOTA	1532	С	GLY B	76	11.570	14.981	56.751	1.00 21.83	С
	MOTA	1533	0	GLY B	76	10.769	15.857	57.076	1.00 19.87	0
	MOTA	1534	N	LEU B	77	11.655	14.508	55.505	1.00 20.87	N
	MOTA	1535	CA	LEU B	77	10.820	15.038	54.433	1.00 19.22	С
	MOTA	1536	СВ	LEU B	77	11.679	15.795	53.418	1.00 19.77	С
25	MOTA	1537	CG	LEU B	77	12.495	17.003	53.873	1.00 21.45	С

	MOTA	1538	CD1	LEU B	77	13.547	17.334	52.816	1.00 23.98	С
	MOTA	1539	CD2	LEU B	77	11.577	18.164	54.122	1.00 17.71	С
	MOTA	1540	С	LEU B	77	9.981	14.022	53.657	1.00 20.65	C
	MOTA	1541	0	LEU B	77	10.445	12.943	53.291	1.00 20.00	0
5	MOTA	1542	N	ASN B	78	8.731	14.392	53.410	1.00 19.49	N
	MOTA	1543	CA	ASN B	78	7.822	13.577	52.629	1.00 19.83	С
	MOTA	1544	СВ	ASN B	78	6.382	13.725	53.137	1.00 20.64	С
	MOTA	1545	CG	ASN B	78	5.973	12.637	54.111	1.00 21.67	С
	MOTA	1546	OD1	ASN B	78	6.799	11.869	54.604	1.00 18.96	0
10	MOTA	1547	ND2	ASN B	78	4.679	12.575	54.398	1.00 16.01	N
	MOTA	1548	С	ASN B	78	7.923	14.203	51.241	1.00 19.96	С
	MOTA	1549	0	ASN B	78	7.819	15.424	51.106	1.00 21.03	0
	ATOM	1550	N	LEU B	79	8.154	13.379	50.227	1.00 19.97	N
	MOTA	1551	CA	LEU B	79	8.243	13.857	48.855	1.00 20.38	С
15	MOTA	1552	CB	LEU B	79	9.607	13.528	48.224	1.00 21.06	С
	MOTA	1553	CG	LEU B	79	10.830	14.410	48.503	1.00 20.33	С
	ATOM	1554	CD1	LEU B	79	11.176	14.376	49.981	1.00 15.77	С
	MOTA	1555	CD2	LEU B	79	12.006	13.919	47.655	1.00 25.25	С
	MOTA	1556	С	LEU B	79	7.153	13.157	48.055	1.00 21.10	С
20	ATOM	1557	0	LEU B	79	7.196	11.938	47.865	1.00 20.88	0
	MOTA	1558	N	THR B	80	6.164	13.926	47.609	1.00 20.87	N
	MOTA	1559	CA	THR B	80	5.086	13.365	46.810	1.00 20.85	С
	ATOM	1560	СВ	THR B	80	3.702	13.899	47.273	1.00 20.49	С
	MOTA	1561	OG1	THR B	80	3.477	13.532	48.643	1.00 20.65	0
25	ATOM	1562	CG2	THR B	80	2.587	13.314	46.415	1.00 19.59	С

MOTA	1563	С	THR B	80	5.363	13.783	45.370	1.00 20.80	С
MOTA	1564	О	THR B	80	5.304	14.963	45.037	1.00 20.97	0
MOTA	1565	N	SER B	81	5.691	12.816	44.525	1.00 21.75	N
MOTA	1566	CA	SER B	81	6.002	13.107	43.132	1.00 22.99	С
MOTA	1567	СВ	SER B	81	7.352	12.494	42.752	1.00 22.82	С
MOTA	1568	OG	SER B	81	8.418	13.029	43.522	1.00 27.07	О
MOTA	1569	С	SER B	81	4.951	12.612	42.145	1.00 24.46	С
MOTA	1570	0	SER B	81	4.392	11.514	42.285	1.00 24.48	0
MOTA	1571	N	THR B	82	4.688	13.445	41.147	1.00 25.52	N
MOTA	1572	CA	THR B	82	3.744	13.130	40.085	1.00 26.98	С
MOTA	1573	СВ	THR B	82	2.716	14.253	39.910	1.00 27.26	С
MOTA	1574	OG1	THR B	82	1.968	14.397	41.124	1.00 28.56	Ō
MOTA	1575	CG2	THR B	82	1.768	13.939	38.759	1.00 26.26	С
MOTA	1576	С	THR B	82	4.618	13.023	38.841	1.00 28.72	С
MOTA	1577	0	THR B	82	5.343	13.964	38.507	1.00 28.19	0
MOTA	1578	N	PHE B	83	4.560	11.877	38.166	1.00 30.09	N
MOTA	1579	CA	PHE B	83	5.385	11.659	36.989	1.00 33.13	С
MOTA	1580	СВ	PHE B	83	6.702	11.011	37.408	1.00 33.32	С
MOTA	1581	CG	PHE B	83	6.532	9.719	38.164	1.00 35.08	С
MOTA	1582	CD1	PHE B	83	6.000	9.710	39.452	1.00 35.79	С
MOTA	1583	CE1	PHE B	83	5.858	8.515	40.160	1.00 37.06	С
MOTA	1584	CZ	PHE B	83	6.250	7.309	39.580	1.00 35.12	С
MOTA	1585	CE2	PHE B	83	6.780	7.305	38.297	1.00 34.32	С
MOTA	1586	CD2	PHE B	83	6.919	8.508	37.595	1.00 35.78	С
MOTA	1587	С	PHE B	83	4.736	10.807	35.904	1.00 35.08	С
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	ATOM 1564 ATOM 1565 ATOM 1566 ATOM 1567 ATOM 1568 ATOM 1569 ATOM 1571 ATOM 1572 ATOM 1573 ATOM 1574 ATOM 1575 ATOM 1576 ATOM 1576 ATOM 1577 ATOM 1578 ATOM 1578 ATOM 1578 ATOM 1580 ATOM 1581 ATOM 1582 ATOM 1583 ATOM 1584 ATOM 1585 ATOM 1585	ATOM 1564 O ATOM 1565 N ATOM 1566 CA ATOM 1567 CB ATOM 1568 OG ATOM 1569 C ATOM 1571 N ATOM 1572 CA ATOM 1573 CB ATOM 1574 OG1 ATOM 1575 CG2 ATOM 1576 C ATOM 1577 O ATOM 1577 O ATOM 1578 N ATOM 1578 N ATOM 1579 CA ATOM 1580 CB ATOM 1580 CB ATOM 1581 CG ATOM 1582 CD1 ATOM 1583 CE1 ATOM 1584 CZ ATOM 1585 CE2 ATOM 1586 CD2	ATOM 1564 O THR B ATOM 1565 N SER B ATOM 1566 CA SER B ATOM 1567 CB SER B ATOM 1568 OG SER B ATOM 1569 C SER B ATOM 1570 O SER B ATOM 1571 N THR B ATOM 1572 CA THR B ATOM 1573 CG THR B ATOM 1574 OG THR B ATOM 1577 O THR B ATOM 1577 O THR B ATOM 1577 O THR B ATOM 1578 N PHE B ATOM 1580 CB PHE B ATOM 1581 CG PHE B ATOM 1582 CD PHE B ATOM 1584 CZ PHE B ATOM 1585 CE2 PHE B ATOM 1586 CE2 PHE B	ATOM 1564 O THR B 80 ATOM 1565 N SER B 81 ATOM 1566 CA SER B 81 ATOM 1569 C SER B 81 ATOM 1570 CA THR B 82 ATOM 1571 CA THR B 82 ATOM 1574 CA THR B 82 ATOM 1574 CA THR B 82 ATOM 1575 CG2 THR B 82 ATOM 1576 CA THR B 82 ATOM 1577 CA THR B 82 ATOM 1577 CA THR B 82 ATOM 1577 CA THR B 82 ATOM 1578 N PHE B 83 ATOM 1580 CB PHE B 83 ATOM 1580 CB PHE B 83 ATOM 1581 CG2 PHE B 83 ATOM 1581 CG2 PHE B 83 ATOM 1582 CG2 PHE B 83 ATOM 1582 CG2 PHE B 83 ATOM 1583 CG2 PHE B 83 ATOM 1584 CG2 PHE B 83 ATOM 1584 CG2 PHE B 83 ATOM 1585 CG2 PHE B 83 ATOM 1586 CG2 PHE B 8	ATOM 1564 O THR B 80 5.304 ATOM 1566 IN SER B 81 5.691 ATOM 1566 CA SER B 81 7.352 ATOM 1567 CB SER B 81 7.352 ATOM 1568 OG SER B 81 8.418 ATOM 1569 C SER B 81 4.951 ATOM 1570 O SER B 81 4.392 ATOM 1571 N THR B 82 4.688 ATOM 1572 CA THR B 82 2.716 ATOM 1573 CB THR B 82 2.716 ATOM 1574 OG THR B 82 1.968 ATOM 1575 CG2 THR B 82 1.768 ATOM 1577 O THR B 82 1.768 ATOM 1578 N PHE B 83 4.560 ATOM 1580 CB PHE B 83 6.702 ATOM 1581 CG PHE B 83 6.702 ATOM 1582 CD1 PHE B 83 6.250 ATOM 1584 CZ PHE B 83 6.780 ATOM 1585 CE2 PHE B 83 6.780 ATOM 1586 CD2 PHE B 83 6.780	ATOM 1564 O THR B 80 5.304 14.963 ATOM 1566 CA SER B 81 5.691 12.816 ATOM 1566 CA SER B 81 6.002 13.107 ATOM 1567 CB SER B 81 7.352 12.494 ATOM 1568 OG SER B 81 8.418 13.029 ATOM 1569 C SER B 81 4.951 12.612 ATOM 1570 O SER B 81 4.991 11.514 ATOM 1571 N THR B 82 4.688 13.445 ATOM 1572 CA THR B 82 3.744 13.130 ATOM 1573 CB THR B 82 1.968 14.397 ATOM 1574 OG1 THR B 82 1.968 14.397 ATOM 1575 CG2 THR B 82 1.968 14.397 ATOM 1576 C THR B 82 1.968 13.939 ATOM 1577 O THR B 82 1.968 13.939 ATOM 1578 N FHE B 82 1.768 13.923 ATOM 1578 CB THR B 82 1.768 13.923 ATOM 1579 CA FHE B 83 4.560 11.877 ATOM 1580 CB FHE B 83 6.702 11.011 ATOM 1581 CG FHE B 83 6.702 11.011 ATOM 1582 CD FHE B 83 6.702 9.719 ATOM 1583 CE FHE B 83 6.702 9.719 ATOM 1584 CF FHE B 83 6.702 7.309 ATOM 1585 CE FHE B 83 6.700 7.309 ATOM 1584 CF FHE B 83 6.700 7.309 ATOM 1585 CE FHE B 83 6.780 7.309 ATOM 1584 CF FHE B 83 6.780 7.309	ATOM 1564 O THR B 80 5.304 14.963 45.037 ATOM 1565 N SER B 81 5.691 12.816 44.525 ATOM 1566 CA SER B 81 6.002 13.107 43.132 ATOM 1567 CB SER B 81 7.352 12.494 42.752 ATOM 1569 C SER B 81 8.418 13.029 43.522 ATOM 1569 C SER B 81 4.951 12.612 42.145 ATOM 1570 O SER B 81 4.392 11.514 42.285 ATOM 1571 N THR B 82 4.688 13.445 41.147 ATOM 1572 CA THR B 82 3.744 13.130 40.085 ATOM 1573 CB THR B 82 2.716 14.253 39.910 ATOM 1574 CJ THR B 82 2.716 14.253 39.910 ATOM 1575 CG THR B 82 1.968 13.939 38.759 ATOM 1576 C THR B 82 1.968 13.939 38.759 ATOM 1577 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 82 1.968 13.939 38.759 ATOM 1578 C THR B 83 6.360 11.877 38.166 ATOM 1580 C THE B 83 6.702 11.011 37.408 ATOM 1582 C THE B 83 6.702 9.719 38.164 ATOM 1582 C THE B 83 6.000 9.710 39.452 ATOM 1584 C THE B 83 6.250 7.309 39.580 ATOM 1584 C THE B 83 6.250 7.309 39.580 ATOM 1584 C THE B 83 6.250 7.309 39.580 ATOM 1586 C THE B 83 6.780 7.309 39.580	ATOM 1564 O THR B 80 5.304 14.963 45.037 1.00 20.97 ATOM 1565 N SER B 81 5.691 12.816 44.525 1.00 21.75 ATOM 1566 CA SER B 81 6.002 13.107 43.132 1.00 22.89 ATOM 1567 CB SER B 81 7.352 12.494 42.752 1.00 22.82 ATOM 1568 CG SER B 81 8.418 13.029 43.522 1.00 27.07 ATOM 1569 C SER B 81 4.951 12.612 42.145 1.00 24.46 ATOM 1570 O SER B 81 4.392 11.514 42.285 1.00 24.48 ATOM 1571 N THR B 82 4.688 13.445 41.147 1.00 25.52 ATOM 1573 CB THR B 82 3.744 13.130 40.085 1.00 26.98 ATOM 1574 CG THR B 82 1.968 14.397 41.124 1.00 28.726 ATOM 1575 CG THR B 82 1.768 13.939 38.759 1.00 28.726 ATOM 1576 C THR B 82 1.668 13.939 38.759 1.00 28.72 ATOM 1577 O THR B 82 1.668 13.939 38.759 1.00 28.72 ATOM 1578 CG THR B 82 1.668 13.939 38.759 1.00 28.72 ATOM 1578 CG THR B 82 1.668 13.939 38.759 1.00 28.72 ATOM 1578 CG THR B 82 1.668 13.939 38.759 1.00 28.72 ATOM 1578 C THR B 83 4.660 11.877 38.166 1.00 30.09 ATOM 1580 CG PHE B 83 6.702 11.011 37.408 1.00 33.33 ATOM 1580 CG PHE B 83 6.000 9.710 39.452 1.00 35.08 ATOM 1583 CEJ PHE B 83 6.000 9.710 39.452 1.00 35.08 ATOM 1584 CZ PHE B 83 6.250 7.309 39.580 1.00 35.08 ATOM 1584 CZ PHE B 83 6.280 7.305 38.297 1.00 35.78 ATOM 1585 CEZ PHE B 83 6.780 7.305 38.297 1.00 34.32 ATOM 1586 CEZ PHE B 83 6.780 7.305 38.297 1.00 34.32

	MOTA	1588	0	PHE B	83	3.757	10.104	36.145	1.00 35.20	0
	MOTA	1589	N	LEU B	84	5.300	10.888	34.703	1.00 37.29	N
	MOTA	1590	CA	LEU B	84	4.827	10.126	33.552	1.00 39.17	С
	MOTA	1591	СВ	LEU B	84	5.018	10.947	32.273	1.00 38.63	С
5	MOTA	1592	CG	LEU B	84	4.592	10.337	30.934	1.00 37.74	С
	MOTA	1593	CD1	LEU B	84	3.086	10.104	30.921	1.00 36.04	С
	MOTA	1594	CD2	LEU B	84	4.997	11.274	29.806	1.00 35.51	С
	MOTA	1595	С	LEU B	84	5.663	8.847	33.485	1.00 40.90	С
	MOTA	1596	0	LEU B	84	6.877	8.911	33.298	1.00 40.46	0
10	MOTA	1597	N	ARG B	85	5.014	7.696	33.651	1.00 43.31	N
	ATOM	1598	CA	ARG B	85	5.705	6.404	33.628	1.00 46.39	С
	MOTA	1599	СВ	ARG B	85	5.027	5.426	34.582	1.00 46.96	С
	ATOM	1600	CG	ARG B	85	5.722	4.082	34.680	1.00 47.76	С
	ATOM	1601	CD	ARG B	85	6.855	4.137	35.685	1.00 50.67	.C
15	MOTA	1602	NE	ARG B	85	7.456	2.829	35.941	1.00 52.88	N
	MOTA	1603	CZ	ARG B	85	6.776	1.731	36.263	1.00 55.13	C
	MOTA	1604	NH1	ARG B	85	5.451	1.761	36.367	1.00 55.46	N
	MOTA	1605	NH2	ARG B	85	7.425	0.598	36.499	1.00 54.74	N
	ATOM	1606	С	ARG B	85	5.710	5.788	32.237	1.00 48.35	С
20	MOTA	1607	0	ARG B	85	6.766	5.559	31.646	1.00 49.00	0
	MOTA	1608	N	LYS B	86	4.514	5.500	31.735	1.00 49.68	N
	MOTA	1609	CA	LYS B	86	4.346	4.913	30.414	1.00 50.77	С
	MOTA	1610	СВ	LYS B	86	4.293	3.390	30.521	1.00 50.85	С
	MOTA	1611	CG	LYS B	86	5.499	2.811	31.242	1.00 52.18	С
25	MOTA	1612	CD	LYS B	86	5.446	1.302	31.337	1.00 55.10	С

	MOTA	1613	CE	LYS B	86	6.667	0.775	32.067	1.00 56.19	C
	MOTA	1614	NZ	LYS B	86	6.681	-0.709	32.134	1.00 54.56	N
	MOTA	1615	С	LYS B	86	3.038	5.457	29.872	1.00 51.30	С
	MOTA	1616	0	LYS B	86	2.026	4.760	29.839	1.00 51.59	0
5	MOTA	1617	N	ASN B	87	3.072	6.720	29.460	1.00 51.82	N
	MOTA	1618	CA	ASN B	87	1.896	7.397	28.939	1.00 52.40	С
	MOTA	1619	СВ	ASN B	87	1.362	6.700	27.685	1.00 53.21	С
	MOTA	1620	CG	ASN B	87	2.156	7.048	26.445	1.00 54.72	С
	MOTA	1621	OD1	ASN B	87	3.274	6.565	26.247	1.00 56.95	0
10	MOTA	1622	ND2	ASN B	87	1.587	7.905	25.605	1.00 55.62	N
	MOTA	1623	С	ASN B	87	0.814	7.449	30.001	1.00 51.79	C
	MOTA	1624	0	ASN B	87	-0.375	7.490	29.688	1.00 52.58	0
	MOTA	1625	N	GLN B	88	1.235	7.437	31.261	1.00 51.17	N
	MOTA	1626	CA	GLN B	88	0.303	7.511	32.380	1.00 50.52	C
15	MOTA	1627	СВ	GLN B	88	-0.030	6.124	32.940	1.00 50.99	С
	MOTA	1628	CG	GLN B	88	-1.045	6.212	34.090	1.00 52.80	C
	MOTA	1629	CD	GLN B	88	-1.101	4.976	34.971	1.00 55.25	С
	MOTA	1630	OE1	GLN B	88	-0.099	4.567	35.561	1.00 54.92	0
	MOTA	1631	NE2	GLN B	88	-2.285	4.382	35.076	1.00 55.03	N
20	MOTA	1632	С	GLN B	88	0.882	8.350	33.512	1.00 49.33	С
	MOTA	1633	0	GLN B	88	2.079	8.292	33.792	1.00 48.79	0
	MOTA	1634	N	CYS B	89	0.025	9.129	34.161	1.00 48.09	N
	MOTA	1635	CA	CYS B	89	0.451	9.956	35.278	1.00 47.25	С
	MOTA	1636	СВ	CYS B	89	-0.463	11.173	35.441	1.00 47.96	С
25	MOTA	1637	SG	CYS B	89	-0.440	12.321	34.033	1.00 52.30	S

	MOTA	1638	С	CYS B	89	0.417	9.134	36.557	1.00 45.36	С
	MOTA	1639	0	CYS B	89	-0.634	8.637	36.961	1.00 45.21	0
	MOTA	1640	N	GLU B	90	1.573	8.986	37.187	1.00 42.70	N
	MOTA	1641	CA	GLU B	90	1.662	8.234	38.423	1.00 41.56	С
5	MOTA	1642	СВ	GLU B	90	2.663	7.085	38.283	1.00 41.43	С
	MOTA	1643	CG	GLU B	90	2.074	5.833	37.660	1.00 45.26	С
	MOTA	1644	CD	GLU B	90	3.097	4.728	37.493	1.00 48.56	С
	MOTA	1645	OE1	GLU B	90	3.894	4.508	38.430	1.00 49.59	0
	MOTA	1646	OE2	GLU B	90	3.099	4.071	36.430	1.00 50.95	0
10	MOTA	1647	С	GLU B	90	2.075	9.146	39.564	1.00 40.06	C
•	ATOM	1648	0	GLU B	90	2.608	10.234	39.347	1.00 39.58	0
	MOTA	1649	N	THR B	91	1.809	8.697	40.781	1.00 37.76	N
	MOTA	1650	CA	THR B	91	2.159	9.455	41.964	1.00 37.06	С
	MOTA	1651	СВ	THR B	91	0.922	10.101	42.610	1.00 37.34	С
15	MOTA	1652	OG1	THR B	91	0.602	11.308	41.908	1.00 37.99	0
	MOTA	1653	CG2	THR B	91	1.180	10.428	44.069	1.00 36.87	С
	MOTA	1654	С	THR B	91	2.815	8.524	42.956	1.00 35.97	С
	MOTA	1655	0	THR B	91	2.307	7.442	43.234	1.00 36.79	0
	MOTA	1656	N	LYS B	92	3.961	8.942	43.470	1.00 34.66	N
20	MOTA	1657	CA	LYS B	. 92	4.670	8.141	44.442	1.00 34.25	С
	MOTA	1658	СВ	LYS B	92	5.930	7.526	43.823	1.00 35.39	С
	MOTA	1659	CG	LYS B	92	6.573	6.473	44.724	1.00 40.91	С
	MOTA	1660	CD	LYS B	92	7.770	5.797	44.073	1.00 47.37	С
	MOTA	1661	CE	LYS B	92	8.295	4.668	44.950	1.00 49.29	С
25	MOTA	1662	NZ	LYS B	92	9.460	3.958	44.346	1.00 51.25	N

	MOTA	1663	С	LYS B	92	5.047	9.016	45.624	1.00 32.07	С
	MOTA	1664	0	LYS B	92	5.201	10.229	45.492	1.00 31.59	0
	MOTA	1665	N	ILE B	93	5.177	8.394	46.787	1.00 30.05	N
	MOTA	1666	CA	ILE B	93	5.564	9.110	47.986	1.00 29.86	С
5	MOTA	1667	СВ	ILE B	93	4.489	9.004	49.082	1.00 28.91	С
	MOTA	1668	CG1	ILE B	93	3.221	9.726	48.619	1.00 29.22	С
	MOTA	1669	CD1	ILE B	93	2.075	9.651	49.590	1.00 33.59	С
	MOTA	1670	CG2	ILE B	93	5.006	9.615	50.381	1.00 31.24	С
	MOTA	1671	С	ILE B	93	6.865	8.524	48.500	1.00 29.02	С
10	MOTA	1672	0	ILE B	93	6.973	7.314	48.697	1.00 29.59	0
	MOTA	1673	N	MET B	94	7.855	9.389	48.683	1.00 28.74	N
	ATOM	1674	CA	MET B	94	9.157	8.982	49.192	1.00 28.69	С
	ATOM	1675	СВ	MET B	94	10.268	9.380	48.223	1.00 30.16	С
	ATOM	1676	CG	MET B	94	10.133	8.774	46.852	1.00 33.76	С
15	MOTA	1677	SD	MET B	94	11.342	9.469	45.713	1.00 42.95	S
	MOTA	1678	CE	MET B	94	12.813	8.613	46.225	1.00 39.86	С
	MOTA	1679	С	MET B	94	9.386	9.693	50.519	1.00 26.85	С
	MOTA	1680	0	MET B	94	9.071	10.879	50.671	1.00 26.13	0
	MOTA	1681	N	VAL B	95	9.938	8.962	51.477	1.00 24.54	N
20	MOTA	1682	CA	VAL B	95	10.222	9.525	52.781	1.00 23.92	С
	MOTA	1683	СВ	VAL B	95	9.664	8.653	53.915	1.00 23.21	С
	MOTA	1684	CG1	VAL B	95	10.142	9.197	55.253	1.00 23.76	С
	MOTA	1685	CG2	VAL B	95	8.133	8.611	53.859	1.00 26.68	С
	MOTA	1686	С	VAL B	95	11.725	9.645	53.001	1.00 23.60	С
25	MOTA	1687	0	VAL B	95	12.438	8.639	53.039	1.00 24.63	0

	MOTA	1688	N	LEU B	96	12.199	10.880	53.122	1.00 23.77	N
	MOTA	1689	CA	LEU B	96	13.605	11.130	53.408	1.00 24.17	С
	MOTA	1690	СВ	LEU B	96	14.077	12.432	52.762	1.00 24.53	С
	MOTA	1691	CG	LEU B	96	14.079	12.475	51.231	1.00 26.20	С
5	ATOM	1692	CD1	LEU B	96	14.585	13.838	50.746	1.00 29.41	С
	ATOM	1693	CD2	LEU B	96	14.956	11.368	50.693	1.00 26.73	С
	MOTA	1694	С	LEU B	96	13.682	11.241	54.926	1.00 23.73	С
	ATOM	1695	0	LEU B	96	13.213	12.221	55.516	1.00 22.46	0
	ATOM	1696	N	GLN B	97	14.250	10.213	55.550	1.00 25.09	N
10	ATOM	1697	CA	GLN B	97	14.396	10.160	56.996	1.00 26.98	С
	ATOM	1698	СВ	GLN B	97	14.563	8.703	57.446	1.00 28.85	С
	ATOM	1699	CG	GLN B	97	13.516	8.208	58.442	1.00 37.81	С
	ATOM	1700	CD	GLN B	97	12.180	7.884	57.798	1.00 46.93	С
	MOTA	1701	OE1	GLN B	97	12.107	7.113	56.840	1.00 52.64	0
15	ATOM	1702	NE2	GLN B	97	11.116	8.464	58.329	1.00 50.81	N
	ATOM	1703	С	GLN B	97	15.611	10.969	57.433	1.00 26.07	С
	ATOM	1704	0	GLN B	97	16.664	10.901	56.811	1.00 25.85	0
	MOTA	1705	N	PRO B	98	15.489	11.725	58.533	1.00 27.95	N
	MOTA	1706	CA	PRO B	98	16.634	12.522	58.991	1.00 28.20	С
20	MOTA	1707	СВ	PRO B	98	16.143	13.128	60.310	1.00 27.26	С
	MOTA	1708	CG	PRO B	98	14.649	12.996	60.249	1.00 31.44	С
	MOTA	1709	CD	PRO B	98	14.448	11.672	59.567	1.00 26.47	С
	MOTA	1710	C·	PRO B	98	17.848	11.616	59.204	1.00 28.83	С
	ATOM	1711	0	PRO B	98	17.701	10.470	59.647	1.00 30.17	0
25	MOTA	1712	N	ALA B	99	19.041	12.124	58.902	1.00 28.42	N

	MOTA	1713	CA	ALA B 99	20.254	11.331	59.076	1.00 28.17	С
	ATOM	1714	СВ	ALA B 99	20.883	11.034	57.709	1.00 26.53	С
	ATOM	1715	С	ALA B 99	21.298	11.954	60.013	1.00 28.73	С
	MOTA	1716	0	ALA B 99	22.477	12.021	59.681	1.00 30.28	0
5	MOTA	1717	N	GLY B 100	20.860	12.424	61.174	1.00 30.15	N
	ATOM	1718	CA	GLY B 100	21.788	12.988	62.143	1.00 30.98	С
	ATOM	1719	С	GLY B 100	22.332	14.399	61.954	1.00 32.27	С
	ATOM	1720	0	GLY B 100	23.053	14.891	62.833	1.00 32.39	0
	MOTA	1721	N	ALA B 101	22.005	15.050	60.836	1.00 30.10	N
10	MOTA	1722	CA	ALA B 101	22.483	16.407	60.575	1.00 28.93	С
	MOTA	1723	СВ	ALA B 101	23.926	16.364	60.098	1.00 29.35	С
	MOTA	1724	С	ALA B 101	21.616	17.136	59.546	1.00 27.78	С
	MOTA	1725	0	ALA B 101	21.133	16.536	58.587	1.00 27.81	0
	MOTA	1726	N	PRO B 102	21.428	18.455	59.724	1.00 27.63	N
15	MOTA	1727	CA	PRO B 102	20.606	19.232	58.789	1.00 27.52	С
	MOTA	1728	CB	PRO B 102	20.770	20.668	59.286	1.00 27.31	С
	MOTA	1729	CG	PRO B 102	21.021	20.482	60.767	1.00 28.49	С
	MOTA	1730	CD	PRO B 102	21.980	19.317	60.785	1.00 27.05	С
	MOTA	1731	С	PRO B 102	21.060	19.069	57.345	1.00 26.25	С
20	ATOM	1732	0	PRO B 102	22.233	19.265	57.034	1.00 26.32	0
	ATOM	1733	N	GLY B 103	20.125	18.706	56.471	1.00 24.95	N
	ATOM	1734	CA	GLY B 103	20.448	18.533	55.066	1.00 23.66	С
	ATOM	1735	С	GLY B 103	20.925	17.135	54.711	1.00 20.21	С
	ATOM	1736	0	GLY B 103	21.343	16.895	53.578	1.00 21.21	0
25	MOTA	1737	N	HIS B 104	20.857	16.218	55.672	1.00 17.17	N

	MOTA	1738	CA	HIS B	104	21.280	14.844	55.451	1.00 19.	.03 C
	MOTA	1739	СВ	HIS B	104	22.481	14.536	56.334	1.00 17.	.66 C
	MOTA	1740	CG	HIS B	104	23.672	15.379	56.015	1.00 21.	.52 C
	MOTA	1741	ND1	HIS B	104	24.690	14.942	55.196	1.00 17.	.48 N
5	MOTA	1742	CE1	HIS B	104	25.546	15.929	55.002	1.00 19.	.71 C
	MOTA	1743	NE2	HIS B	104	25.123	16.987	55.671	1.00 20.	.79 N
	MOTA	1744	CD2	HIS B	104	23.956	16.669	56.318	1.00 19.	.37 C
	MOTA	1745	С	HIS B	104	20.136	13.897	55.747	1.00 16.	.96 C
	MOTA	1746	0	HIS B	104	19.540	13.953	56.810	1.00 16.	73 0
10	MOTA	1747	N	TYR B	105	19.836	13.022	54.795	1.00 19.	61 N
	MOTA	1748	CA	TYR B	105	18.735	12.080	54.945	1.00 21.	.07 C
	MOTA	1749	СВ	TYR B	105	17.532	12.543	54.123	1.00 21.	.53 C
	MOTA	1750	CG	TYR B	105	17.107	13.974	54.357	1.00 21.	91 C
	MOTA	1751	CD1	TYR B	105	16.219	14.302	55.389	1.00 20.	70 C
15	MOTA	1752	CE1	TYR B	105	15.843	15.621	55.616	1.00 22.	27 C
	MOTA	1753	CZ	TYR B	105	16.354	16.636	54.807	1.00 23.	.20 C
	MOTA	1754	ОН	TYR B	105	15.977	17.950	55.020	1.00 23.	16 0
	MOTA	1755	CE2	TYR B	105	17.237	16.335	53.776	1.00 18.	.32 C
	MOTA	1756	CD2	TYR B	105	17.608	15.007	53.555	1.00 21.	.82 C
20	MOTA	1757	С	TYR B	105	19.106	10.698	54.451	1.00 21.	.92 C
	MOTA	1758	0	TYR B	105	20.104	10.514	53.763	1.00 23.	.47 0
	MOTA	1759	N	THR B	106	18.267	9.733	54.790	1.00 24.	.22 N
	MOTA	1760	CA	THR B	106	18.438	8.364	54.333	1.00 26	.64 C
	MOTA	1761	СВ	THR B	106	18.666	7.393	55.504	1.00 25	.91 C
25	MOTA	1762	OG1	THR B	106	17.607	7.541	56.463	1.00 30	.22 0

	MOTA	1763	CG2	THR B 106	20.011	7.689	56.174	1.00 26.89	С
	ATOM	1764	С	THR B 106	17.126	8.029	53.635	1.00 27.69	С
	ATOM	1765	0	THR B 106	16.056	8.487	54.057	1.00 25.39	0
	MOTA	1766	N	TYR B 107	17.214	7.253	52.561	1.00 29.73	N
5	MOTA	1767	CA	TYR B 107	16.038	6.864	51:801	1.00 33.54	С
	MOTA	1768	СВ	TYR B 107	15.924	7.714	50.537	1.00 33.57	С
	MOTA	1769	CG	TYR B 107	15.054	7.073	49.482	1.00 37.64	С
	MOTA	1770	CD1	TYR B 107	13.708	6.794	49.738	1.00 41.90	С
	MOTA	1771	CE1	TYR B 107	12.909	6.159	48.790	1.00 43.55	С
10	MOTA	1772	CZ	TYR B 107	13.459	5.792	47.571	1.00 46.00	С
	MOTA	1773	OH	TYR B 107	12.673	5.158	46.635	1.00 49.14	0
	MOTA	1774	CE2	TYR B 107	14.796	6.060	47.292	1.00 43.74	С
	MOTA	1775	CD2	TYR B 107	15.583	6.702	48.247	1.00 38.84	С
	MOTA	1776	С	TYR B 107	16.061	5.388	51.420	1.00 36.23	С
15	MOTA	1777	0	TYR B 107	17.018	4.899	50.818	1.00 35.45	0
	MOTA	1778	N	SER B 108	14.993	4.681	51.769	1.00 40.28	N
	MOTA	1779	CA	SER B 108	14.877	3.259	51.470	1.00 44.66	С
	MOTA	1780	CB	SER B 108	13.988	2.580	52.506	1.00 44.48	С
	MOTA	1781	OG	SER B 108	13.351	1.451	51.940	1.00 47.59	0
20	MOTA	1782	С	SER B 108	14.306	2.996	50.086	1.00 47.15	С
	MOTA	1783	0	SER B 108	13.296	3.581	49.703	1.00 47.89	0
	ATOM	1784	N	SER B 109	14.943	2.094	49.348	1.00 50.48	N
	MOTA	1785	CA	SER B 109	14.487	1.751	48.007	1.00 53.87	С
	MOTA	1786	СВ	SER B 109	15.609	1.994	46.993	1.00 54.04	С
25	ATOM	1787	œ	SER B 109	15.234	1.547	45.700	1.00 57.33	0

	MOTA	1788	С	SER B 1	09	14.023	0.298	47.920	1.00	55.77	С
	ATOM	1789	0	SER B 1	09	14.760	-0.567	47.445	1.00	55.70	0
	MOTA	1790	N	PRO B 1	10	12.791	0.010	48.379	1.00	57.97	N
	MOTA	1791	CA	PRO B 1	10	12.247	-1.352	48.342	1.00	59.41	C
5	MOTA	1792	СВ	PRO B 1	10	10.771	-1.137	48.658	1.00	59.43	С
	MOTA	1793	CG	PRO B 1	10	10.826	-0.010	49.639	1.00	59.26	С
	MOTA	1794	CD	PRO B 1	10	11.814	0.940	48.977	1.00	58.27	С
	MOTA	1795	С	PRO B 1	10	12.466	-2.035	46.994	1.00	60.89	С
	MOTA	1796	0	PRO B 1	10	12.780	-3.225	46.941	1.00	61.42	0
10	MOTA	1797	N	HIS B 1	11	12.298	-1.279	45.908	1.00	62.25	N
	MOTA	1798	CA	HIS B 1	11	12.501	-1.818	44.564	1.00	63.28	C
	MOTA	1799	СВ	HIS B 1	11	12.336	-0.724	43.502	1.00	64.21	C
	MOTA	1800	CG	HIS B 1	11	10.952	-0.166	43.405	1.00	67.26	С
	MOTA	1801	ND1	HIS B 1	11	10.332	0.482	44.453	1.00	69.85	N
15	MOTA	1802	CE1	HIS B 1	11	9.130	0.877	44.074	1.00 7	0.46	С
	MOTA	1803	NE2	HIS B 1	11	8.946	0.508	42.818	1.00 7	0.26	N
	MOTA	1804	CD2	HIS B 1	11	10.070	-0.146	42.377	1.00	69.17	С
	MOTA	1805	С	HIS B 1	11	13.918	-2.370	44.469	1.00	62.59	С
	MOTA	1806	0	HIS B 1	11	14.148	-3.571	44.615	1.00	63.03	0
20	MOTA	1807	N	SER B 1	12	14.862	-1.466	44.221	1.00	61.45	N
	MOTA	1808	CA	SER B 1	12	16.272	-1.804	44.101	1.00	60.38	С
	MOTA	1809	СВ	SER B 1	12	17.115	-0.527	44.156	1.00	60.82	С
	MOTA	1810	Œ	SER B 1	12	18.482	-0.823	44.399	1.00	62.59	0
	MOTA	1811	С	SER B 1	12	16.730	-2.749	45.200	1.00	58.84	С
25	ATOM	1812	0	SER B 1	12	17.523	-3.661	44.962	1.00	58.90	0

	MOTA	1813	N	GLY B 113	3 16.216	-2.529	46.405	1.00 57.13	N
	MOTA	1814	CA	GLY B 113	3 16.618	-3.346	47.530	1.00 55.12	С
	MOTA	1815	С	GLY B 113	3 17.859	-2.704	48.119	1.00 53.27	С
	MOTA	1816	0	GLY B 113	3 18.847	-3.378	48.414	1.00 52.87	0
5	ATOM	1817	N	SER B 114	17.811	-1.384	48.274	1.00 51.27	N
	MOTA	1818	CA	SER B 114	18.942	-0.654	48.827	1.00 49.51	С
	MOTA	1819	СВ	SER B 114	19.952	-0.353	47.719	1.00 50.16	С
	ATOM	1820	œ	SER B 114	19.337	0.344	46.644	1.00 48.59	0
	ATOM	1821	С	SER B 114	18.548	0.647	49.519	1.00 48.18	С
10	MOTA	1822	0	SER B 114	17.461	1.183	49.296	1.00 48.12	0
	ATOM	1823	N	ILE B 115	5 19.445	1.133	50.372	1.00 46.06	N
	ATOM	1824	CA	ILE B 119	5 19.248	2.383	51.100	1.00 44.42	С
	ATOM	1825	CB	ILE B 115	5 19.600	2.237	52.606	1.00 44.90	С
	ATOM	1826	CG1	ILE B 115	5 18.543	1.394	53.322	1.00 46.80	С
15	ATOM	1827	CD1	ILE B 115	5 17.184	2.066	53.435	1.00 45.52	С
	ATOM	1828	CG2	ILE B 119	5 19.687	3.610	53.261	1.00 46.02	С
	MOTA	1829	С	ILE B 11	5 20.189	3.412	50.480	1.00 41.86	С
	MOTA	1830	0	ILE B 119	5 21.241	3.060	49.949	1.00 41.37	0
	ATOM	1831	N	HIS B 116	5 19.799	4.681	50.534	1.00 39.40	N
20	ATOM	1832	CA	HIS B 110	20.613	5.749	49.974	1.00 36.16	С
	MOTA	1833	СВ	HIS B 11	5 19.902	6.413	48.783	1.00 36.63	С
	ATOM	1834	CG	HIS B 110	6 19.458	5.460	47.714	1.00 37.67	С
	MOTA	1835	ND1	HIS B 110	6 18.918	5.892	46.519	1.00 41.47	N
	MOTA	1836	CE1	HIS B 110	6 18.570	4.847	45.790	1.00 40.60	С
25	MOTA	1837	NE2	HIS B 11	6 18.867	3.752	46.466	1.00 38.98	N

	MOTA	1838	CD2	HIS	В 116	19.426	4.109	47.671	1.00 39.98	С
	MOTA	1839	С	HIS	В 116	20.874	6.810	51.037	1.00 33.97	С
	MOTA	1840	0	HIS	в 116	20.077	6.991	51.954	1.00 32.57	0
	MOTA	1841	N	SER	в 117	22.003	7.498	50.908	1.00 31.18	N
5	MOTA	1842	CA	SER	в 117	22.379	8.564	51.828	1.00 30.38	С
	MOTA	1843	СВ	SER.	в 117	23.787	8.339	52.382	1.00 28.97	С
	MOTA	1844	OG	SER	в 117	23.801	7.236	53.268	1.00 35.19	0
	MOTA	1845	С	SER	в 117	22.336	9.840	51.009	1.00 28.86	С
	ATOM	1846	0	SER	в 117	23.181	10.058	50.139	1.00 28.75	0
10	MOTA	1847	N	VAL	в 118	21.344	10.677	51.293	1.00 27.21	N
	MOTA	1848	CA	VAL	в 118	21.139	11.920	50.555	1.00 24.78	С
	MOTA	1849	СВ	VAL	в 118	19.634	12.130	50.259	1.00 24.46	С
	ATOM	1850	CG1	VAL	в 118	19.417	13.417	49.484	1.00 25.74	С
	ATOM	1851	CG2	VAL	В 118	19.093	10.944	49.492	1.00 28.06	С
15	MOTA	1852	С	VAL	в 118	21.644	13.155	51.281	1.00 24.11	С
	MOTA	1853	0	VAL	в 118	21.399	13.338	52.469	1.00 23.10	0
	ATOM	1854	N	SER	в 119	22.346	14.011	50.551	1.00 23.66	N
	MOTA	1855	CA	SER	в 119	22.838	15.238	51.135	1.00 23.20	С
	MOTA	1856	СВ	SER	в 119	24.342	15.125	51.435	1.00 23.15	С
20	ATOM	1857	œ	SER	в 119	25.095	14.833	50.271	1.00 27.22	0
	ATOM	1858	С	SER	в 119	22.563	16.397	50.188	1.00 21.37	С
	MOTA	1859	0	SER	в 119	22.489	16.216	48.978	1.00 20.94	0
	MOTA	1860	N	VAL	в 120	22.364	17.582	50.756	1.00 22.48	N
	MOTA	1861	CA	VAL	в 120	22.134	18.784	49.966	1.00 21.59	С
25	MOTA	1862	СВ	VAL	в 120	21.263	19.802	50.726	1.00 23.28	С

	MOTA	1863	CG1	VAL B	120	21.150	21.090	49.926	1.00	20.40	C
	MOTA	1864	CG2	VAL B	120	19.861	19.218	50.963	1.00	23.55	С
	MOTA	1865	С	VAL B	120	23.509	19.397	49.718	1.00	21.37	С
	MOTA	1866	0	VAL B	120	24.131	19.938	50.628	1.00	20.79	.0
5	MOTA	1867	N	VAL B	121	23.990	19.297	48.488	1.00	20.82	N
	MOTA	1868	CA	VAL B	121	25.299	19.838	48.147	1.00	18.66	С
	MOTA	1869	СВ	VAL B	121	25.717	19.392	46.738	1.00	19.78	С
	MOTA	1870	CG1	VAL B	121	27.081	20.006	46.358	1.00	20.77	С
	MOTA	1871	CG2	VAL B	121	25.759	17.882	46.681	1.00	22.61	С
10	MOTA	1872	С	VAL B	121	25.274	21.362	48.192	1.00	18.80	С
	MOTA	1873	0	VAL B	121	26.117	22.005	48.825	1.00	15.52	0
	MOTA	1874	N	GLU B	122	24.285	21.931	47.524	1.00	18.78	N
•	MOTA	1875	CA	GLU B	122	24.139	23.376	47.447	1.00	20.84	С
	MOTA	1876	СВ	GLU B	122	25.021	23.914	46.321	1.00	20.82	C
15	MOTA	1877	CG	GLU B	122	25.154	25.410	46.270	1.00	23.89	С
	MOTA	1878	CD	GLU B	122	26.095	25.847	45.169	1.00	28.52	С
	MOTA	1879	OE1	GLU B	122	25.625	26.400	44.154	1.00	31.82	0
	MOTA	1880	OE2	GLU B	122	27.311	25.618	45.314	1.00	29.06	0
	MOTA	1881	С	GLU B	122	22.684	23.665	47.132	1.00	20.92	С
20	MOTA	1882	0	GLU B	122	22.026	22.865	46.460	1.00	20.92	0
	MOTA	1883	N	ALA B	123	22.177	24.805	47.593	1.00	22.15	N
	MOTA	1884	CA	ALA B	123	20.780	25.130	47.333	1.00	23.57	С
	ATOM	1885	СВ	ALA B	123	19.876	24.114	48.050	1.00	21.65	С
	ATOM	1886	С	ALA B	123	20.361	26.545	47.714	1.00	24.94	С
25	ATOM	1887	0	ALA B	123	20.909	27.143	48.633	1.00	27.17	0

	MOTA	1888	N	ASN B	124	19.380	27.056	46.975	1.00	25.25	N
	MOTA	1889	CA	ASN B	124	18.770	28.374	47.181	1.00	25.20	С
	MOTA	1890	СВ	ASN B	124	19.054	29.306	46.003	1.00	25.23	C
	MOTA	1891	CG	ASN B	124	18.413	30.663	46.180	1.00	29.26	C
5	MOTA	1892	OD1	ASN B	124	17.257	30.770	46.594	1.00	26.62	0
	MOTA	1893	ND2	ASN B	124	19.158	31.715	45.854	1.00	32.85	N
	MOTA	1894	С	ASN B	124	17.288	28.034	47.191	1.00	23.20	С
	MOTA	1895	0	ASN B	124	16.723	27.733	46.149	1.00	21.33	0
	MOTA	1896	N	TYR B	125	16.657	28.088	48.359	1.00	23.13	N
10	MOTA	1897	CA	TYR B	125	15.259	27.704	48.475	1.00	24.00	С
	MOTA	1898	СВ	TYR B	125	14.801	27.806	49.934	1.00	25.22	С
	MOTA	1899	CG	TYR B	125	15.077	29.124	50.607	1.00	28.94	С
	MOTA	1900	CD1	TYR B	125	14.295	30.247	50.338	1.00	31.58	С
	MOTA	1901	CE1	TYR B	125	14.559	31.469	50.950	1.00	34.01	С
15	MOTA	1902	CZ	TYR B	125	15.616	31.568	51.836	1.00	34.12	С
	MOTA	1903	ОН	TYR B	125	15.909	32.776	52.421	1.00	38.52	0
	MOTA	1904	CE2	TYR B	125	16.404	30.462	52.123	1.00	34.39	С
	MOTA	1905	ÇD2	TYR B	125	16.131	29.252	51.508	1.00	30.83	С
	MOTA	1906	С	TYR B	125	14.253	28.380	47.551	1.00	24.08	C
20	MOTA	1907	0	TYR B	125	13.123	27.909	47.424	1.00	22.03	0
	MOTA	1908	N	ASP B	126	14.652	29.468	46.900	1.00	23.69	N
	MOTA	1909	CA	ASP B	126	13.753	30.150	45.976	1.00	24.21	С
	MOTA	1910	СВ	ASP B	126	13.891	31.668	46.068	1.00	25.29	С
	MOTA	1911	CG	ASP B	126	13.295	32,230	47.316	1.00	26.34	С
25	ATOM	1912	OD1	ASP B	126	12.139	31.869	47.625	1.00	29.25	0

	MOTA	1913	OD2	ASP B	126	13.985	33.038	47.974	1.00	27.99	0
	MOTA	1914	С	ASP B	126	14.072	29.764	44.554	1.00	25.46	С
	ATOM	1915	0	ASP B	126	13.380	30.180	43.624	1.00	26.59	О
	ATOM	1916	N	GLU B	127	15.124	28.983	44.365	1.00	24.21	N
5	ATOM	1917	CA	GLU B	127	15.502	28.628	43.011	1.00	25.61	С
	MOTA	1918	СВ	GLU B	127	16.654	29.531	42.536	1.00	25.52	С
	ATOM	1919	CG	GLU B	127	16.297	31.019	42.467	1.00	32.98	С
	MOTA	1920	CD	GLU B	127	17.396	31.871	41.838	1.00	39.11	С
	ATOM	1921	OE1	GLU B	127	17.852	31.547	40.719	1.00	41.53	0
10	ATOM	1922	OE2	GLU B	127	17.799	32.875	42.459	1.00	44.56	0
	MOTA	1923	С	GLU B	127	15.870	27.184	42.745	1.00	23.89	С
	ATOM	1924	0	GLU B	127	15.350	26.594	41.805	1.00	23.89	0
	MOTA	1925	N	TYR B	128	16.751	26.603	43.554	1.00	23.39	N
	MOTA	1926	CA	TYR B	128	17.169	25.240	43.274	1.00	22.92	С
15	MOTA	1927	CB.	TYR B	128	18.173	25.266	42.126	1.00	21.87	С
	ATOM	1928	CG	TYR B	128	19.509	25.847	42.552	1.00	24.09	С
	ATOM	1929	CD1	TYR B	128	20.464	25.047	43.182	1.00	22.01	С
	MOTA	1930	CE1	TYR B	128	21.647	25.578	43.659	1.00	24.98	С
	MOTA	1931	CZ	TYR B	128	21.900	26.927	43.511	1.00	26.66	С
20	MOTA	1932	OH	TYR B	128	23.079	27.431	43.998	1.00	30.76	0
	MOTA	1933	CE2	TYR B	128	20.979	27.755	42.885	1.00	29.10	С
	ATOM	1934	CD2	TYR B	128	19.785	27.210	42.405	1.00	23.51	С
	MOTA	1935	С	TYR B	128	17.790	24.506	44.452	1.00	22.50	С
	MOTA	1936	0	TYR B	128	18.143	25.101	45.464	1.00	23.17	0
25	MOTA	1937	N	ALA B	129	17.939	23.196	44.280	1.00	23.06	N

	ATOM	1938	CA	ALA B 129	18.523	22.326	45.281	1.00 22.00	С
	MOTA	1939	СВ	ALA B 129	17.429	21.691	46.143	1.00 22.73	С
•	MOTA	1940	С	ALA B 129	19.300	21.251	44.546	1.00 23.97	С
	ATOM	1941	o ·	ALA B 129	18.751	20.543	43.704	1.00 23.33	0
5	ATOM	1942	N	LEU B 130	20.588	21.154	44.858	1.00 23.49	N
	ATOM	1943	CA	LEU B 130	21.465	20.166	44.250	1.00 24.77	С
	ATOM	1944	СВ	LEU B 130	22.806	20.807	43.893	1.00 24.15	С
	ATOM	1945	CG	LEU B 130	23.789	19.994	43.047	1.00 30.51	С
	ATOM	1946	CD1	LEU B 130	23.151	19.653	41.706	1.00 30.79	С
10	ATOM	1947	CD2	LEU B 130	25.075	20.800	42.840	1.00 28.10	С
	ATOM	1948	С	LEU B 130	21.670	19.060	45.276	1.00 24.21	С
	MOTA	1949	0	LEU B 130	22.287	19.285	46.322	1.00 25.91	0
	ATOM	1950	N	LEU B 131	21.142	17.873	44.982	1.00 24.62	N
	ATOM	1951	CA .	LEU B 131	21.259	16.741	45.894	1.00 24.99	С
15	ATOM	1952	СВ	LEU B 131	19.907	16.062	46.097	1.00 23.32	С
	ATOM	1953	CG	LEU B 131	18.654	16.817	46.533	1.00 27.65	С
	ATOM	1954	CD1	LEU B 131	17.598	15.779	46.854	1.00 27.12	С
	MOTA	1955	CD2	LEU B 131	18.909	17.681	47.747	1.00 24.33	С
	ATOM	1956	С	LEU B 131	22.238	15.681	45.406	1.00 26.69	С
20	MOTA	1957	Ο	LEU B 131	22.398	15.454	44.199	1.00 27.32	0
	MOTA	1958	N	PHE B 132	22.894	15.035	46.362	1.00 26.02	N
	MOTA	1959	CA	PHE B 132	23.820	13.969	46.052	1.00 26.25	С
	MOTA	1960	СВ	PHE B 132	25.237	14.305	46.493	1.00 26.48	C
	ATOM	1961	CG	PHE B 132	26.221	13.193	46.239	1.00 30.21	С
25	ATOM	1962	CD1	PHE B 132	26.596	12.860	44.933	1.00 33.16	С

	MOTA	1963	CE1	PHE B	132	27.476	11.805	44.686	1.00	34.30	C
	MOTA	1964	CZ	PHE B	132	27.992	11.071	45.751	1.00	34.39	С
	MOTA	1965	CE2	PHE B	132	27.629	11.392	47.057	1.00	36.12	С
	MOTA	1966	CD2	PHE B	132	26.746	12.452	47.296	1.00	32.16	С
5	MOTA	1967	С	PHE B	132	23.345	12.750	46.807	1.00	26.32	С
	MOTA	1968	0	PHE B	132	23.065	12.816	48.001	1.00	27.04	0
	MOTA	1969	N	SER B	133	23.231	11.640	46.099	1.00	27.21	N
	MOTA	1970	CA ·	SER B	133	22.802	10.401	46.714	1.00	30.77	С
	MOTA	1971	СВ	SER B	133	21.440	9.993	46.170	1.00	30.65	C,
10	MOTA	1972	OG	SER B	133	21.074	8.721	46.675	1.00	36.04	0
	MOTA	1973	С	SER B	133	23.820	9.294	46.446	1.00	32.06	С
	MOTA	1974	0	SER B	133	24.303	9.123	45.326	1.00	32.43	0
	MOTA	1975	N	ARG B	134	24.169	8.559	47.487	1.00	33.25	N
	MOTA	1976	CA	ARG B	134	25.104	7.465	47.334	1.00	35.64	С
15	MOTA	1977	СВ	ARG B	134	26.446	7.788	48.007	1.00	34.49	С
	MOTA	1978	CG	ARG B	134	26.345	8.228	49.450	1.00	37.30	С
	MOTA	1979	CD	ARG B	134	27.377	9.305	49.764	1.00	38.87	С
	MOTA	1980	NE	ARG B	134	27.331	9.725	51.162	1.00	39.78	N
	MOTA	1981	CZ	ARG B	134	27.740	8.970	52.176	1.00	39.69	С
20	MOTA	1982	NH1	ARG B	134	28.229	7.757	51.945	1.00	42.68	N
	MOTA	1983	NH2	ARG B	134	27.659	9.418	53.420	1.00	36.98	N
	MOTA	1984	С	ARG B	134	24.479	6.221	47.930	1.00	36.40	С
	MOTA	1985	0	ARG B	134	23.870	6.268	49.002	1.00	35.15	0
	MOTA	1986	N	GLY B	135	24.603	5.119	47.198	1.00	38.19	N
25	MOTA	1987	CA	GLY B	135	24.066	3.846	47.642	1.00	41.62	С

	MOTA	1988	С	GLY B 1	L35	25.098	2.763	47.406	1.00	44.13	С
	MOTA	1989	0	GLY B 1	L35	26.115	2.998	46.753	1.00	42.97	О
	MOTA	1990	N	THR B 1	L36	24.844	1.571	47.931	1.00	47.49	N
	MOTA	1991	CA	THR B 1	L36	25.777	0.471	47.764	1.00	50.61	С
5	MOTA	1992	СВ	THR B 1	L36	27.029	0.670	48.632	1.00	51.09	С
	MOTA	1993	OG1	THR B 1	L36	27.838	-0.514	48.580	1.00	52.66	0
	ATOM	1994	CG2	THR B 1	L36	26.635	0.975	50.071	1.00	52.23	С
	MOTA	1995	С	THR B 1	L36	25.148	-0.858	48.131	1.00	52.28	С
	MOTA	1996	0	THR B 1	.36	24.947	-1.158	49.306	1.00	52.60	0
10	MOTA	1997	N	LYS B 1	.37	24.830	-1.651	47.114	1.00	53.62	N
	MOTA	1998	CA	LYS B 1	.37	24.238	-2.964	47.327	1.00	54.93	С
	MOTA	1999	СВ	LYS B 1	.37	23.811	-3.563	45.986	1.00	55.60	С
	ATOM	2000	CG	LYS B 1	.37	22.315	-3.750	45.819	1.00	56.78	С
	MOTA	2001	CD	LYS B 1	.37	21.977	-4.167	44.384	1.00	58.70	С
15	MOTA	2002	CE	LYS B 1	L37	22.698	-5.457	43.978	1.00	58.92	С
	MOTA	2003	NZ	LYS B 1	L 3 7	22.598	-5.762	42.517	1.00	58.82	N
	ATOM	2004	С	LYS B 1	L37	25.245	-3.890	48.007	1.00	55.28	С
	MOTA	2005	0	LYS B 1	L37	24.880	-4.940	48.531	1.00	55.22	0
	MOTA	2006	N	GLY B 1	L38	26.515	-3.490	47.978	1.00	55.65	N
20	MOTA	2007	CA	GLY B 1	L38	27.573	-4.277	48.584	1.00	55.72	С
	MOTA	2008	С	GLY B 1	L38	28.934	-3.779	48.145	1.00	55.93	С
	MOTA	2009	0	GLY B 1	L38	29.019	-2.852	47.334	1.00	55.96	0
	MOTA	2010	N	PRO B 1	L39	30.021	-4.374	48.662	1.00	55.62	N
	MOTA	2011	CA	PRO B 1	L39	31.381	-3.969	48.309	1.00	55.42	С
25	MOTA	2012	СВ	PRO B 1	L39	32.250	-4.922	49.125	1.00	55.83	С

	MOTA	2013	CG	PRO B 13	39 31.4	13 -5.209	50.321	1.00 5	5.60	С
	MOTA	2014	CD	PRO B 13	39 30.0	48 -5.415	49.701	1.00 5	5.87	С
	ATOM	2015	С	PRO B 13	39 31.6	32 -4.044	46.819	1.00 5	4.93	С
•	MOTA	2016	0	PRO B 13	39 32.0	59 -5.092	46.298	1.00 5	6.18	О
5	ATOM	2017	N	GLY B 14	40 31.50	05 -2.920	46.134	1.00 5	3.90	N
	ATOM	2018	CA	GLY B 14	40 31.78	33 -2.864	44.705	1.00 5	2.20	С
	ATOM	2019	С	GLY B 14	40 30.52	27 -2.585	43.913	1.00 5	1.21	С
	ATOM	2020	0	GLY B 14	40 30.5	76 -2.319	42.713	1.00 5	1.38	0
	ATOM	2021	N	GLN B 14	41 29.39	96 -2.665	44.603	1.00 4	9.60	N
10	MOTA	2022	CA	GLN B 14	41 28.10	03 -2.413	43.994	1.00 4	7.90	С
	MOTA	2023	СВ	GLN B 14	41 27.08	35 -3.474	44.431	1.00 4	7.88	С
	MOTA	2024	CĠ	GLN B 14	41 27.32	28 -4.884	43.913	1.00 4	6.95	С
	MOTA	2025 .	CD	GLN B, 14	41 26.23	37 -5.858	44.349	1.00 4	5.80	С
	MOTA	2026	OE1	GLN B 14	41 26.12	26 -6.201	45.522	1.00 4	6.77	0
15	ATOM	2027	NE2	GLN B 14	41 25.42	22 -6.296	43.401	1.00 4	4.27	N
	ATOM	2028	С	GLN B 14	41 27.62	22 -1.030	44.429	1.00 4	6.82	С
	ATOM	2029	0	GLN B 14	41 26.4	10 -0.827	44.695	1.00 4	5.66	0
	ATOM	2030	N	ASN B 14	42 28.5	57 -0.086	44.493	1.00 4	5.91	N
	ATOM	2031	CA	ASN B 14	42 28.2	75 1.284	44.906	1.00 4	4.46	С
20	ATOM	2032	СВ	ASN B 14	42 29.5	1.943	45.455	1.00 4	4.95	С
	MOTA	2033	CG	ASN B 14	42 30.59	93 0.932	45.861	1.00 4	6.96	С
	ATOM	2034	OD1	ASN B 14	42 30.3	73 0.115	46.759	1.00 5	1.35	0
	ATOM	2035	ND2	ASN B 14	42 31.7	45 0.978	45.197	1.00 4	7.04	N
	ATOM	2036	С	ASN B 14	42 27.7	78 2.110	43.740	1.00 4	3.18	С
25	ATOM	2037	0	ASN B 14	42 28.3	72 2.092	42.669	1.00 4	2.88	0

	MOTA	2038	N	PHE B	143	26.689	2.837	43.943	1.00	40.49	N
	MOTA	2039	CA	PHE B	143	26.172	3.688	42.885	1.00	39.21	С
	MOTA	2040	СВ	PHE B	143	24.855	3.120	42.335	1.00	39.22	С
	MOTA	2041	CG	PHE B	143	23.646	3.464	43.147	1.00	41.52	С
5	MOTA	2042	CD1	PHE B	143	23.104	4.743	43.097	1.00	43.86	Ċ
	MOTA	2043	CE1	PHE B	143	21.971	5.063	43.823	1.00	46.05	С
	MOTA	2044	CZ	PHE B	143	21.363	4.097	44.612	1.00	47.94	С
	MOTA	2045	CE2	PHE B	143	21.893	2.813	44.673	1.00	44.88	С
-	MOTA	2046	CD2	PHE B	143	23.029	2.503	43.940	1.00	43.37	С
10	MOTA	2047	С	PHE B	143	25.991	5.110	43.420	1.00	37.46	C
	MOTA	2048	0	PHE B	143	25.731	5.308	44.607	1.00	35.21	0
	MOTA	2049	N	ARG B	144	26.143	6.090	42.537	1.00	35.85	N
	MOTA	2050	CA	ARG B	144	26.013	7.494	42.902	1.00	35.66	С
	MOTA	2051	СВ	ARG B	144	27.356	8.201	42.737	1.00	37.36	С
15	MOTA	2052	CG	ARG B	144	28.516	7.552	43.461	1.00	40.81	С
	MOTA	2053	CD	ARG B	144	29.802	8.273	43.113	1.00	47.7 2	С
	MOTA	2054	NE	ARG B	144	30.956	7.704	43.796	1.00	52.59	N
	MOTA	2055	CZ	ARG B	144	32.207	8.103	43.596	1.00	56.44	С
	MOTA	2056	NH1	ARG B	144	32.461	9.076	42.732	1.00	59.03	N
20	MOTA	2057	NH2	ARG B	144	33.202	7.525	44.254	1.00	58.04	N
	MOTA	2058	С	ARG B	144	24.985	8.207	42.025	1.00	34.31	С
	MOTA	2059	0	ARG B	144	24.860	7.913	40.835	1.00	32.59	0
	MOTA	2060	N	MET B	145	24.260	9.157	42.605	1.00	32.17	N
	MOTA	2061	CA	MET B	145	23.270	9.900	41.842	1.00	31.38	С
25	MOTA	2062	СВ	MET B	145	21.907	9.224	41.957	1.00	32.20	С

	MOTA	2063	CG	MET B 14	45 2	0.805	10.000	41.282	1.00	36.58	C
	MOTA	2064	SD	MET B 14	45 1	.9.260	9.102	41.257	1.00	41.13	S
	MOTA	2065	CE	MET B 14	45 1	.8.612	9.475	42.864	1.00	39.42	С
	MOTA	2066	С	MET B 14	45 2	3.146	11.371	42.239	1.00	30.58	С
5	MOTA	2067	0	MET B 14	45 2	2.959	11.707	43.413	1.00	29.84	0
	MOTA	2068	N	ALA B 14	46 2	3.261	12.241	41.241	1.00	28.92	N
	MOTA	2069	CA	ALA B 14	46 2	3.136	13.681	41.429	1.00	26.73	С
	MOTA	2070	СВ	ALA B 14	4 6 2	4.231	14.409	40.666	1.00	26.72	С
	ATOM	2071	С	ALA B 14	46 2	1.765	14.101	40.904	1.00	26.22	С
10	ATOM	2072	О	ALA B 14	1 6 2	1.378	13.743	39.792	1.00	25.15	0
	ATOM	2073	N	THR B 14	47 2	1.034	14.858	41.712	1.00	26.04	N
	ATOM	2074	CA	THR B 14	47 1	9.707	15.320	41.335	1.00	24.43	С
	MOTA	2075	CB	THR B 14	47 1	8.635	14.690	42.225	1.00	24.48	С
	MOTA	2076	OG1	THR B 14	47 1	8.895	13.287 ⁻	42.346	1.00	28.38	0
15	MOTA	2077	CG2	THR B 14	47 1	7.255	14.891	41.617	1.00	24.67	С
	MOTA	2078	С	THR B 14	47 1	9.606	16.837	41.464	1.00	23.63	С
	MOTA	2079	0	THR B 14	47 2	0.044	17.422	42.462	1.00	22.67	0
	ATOM	2080	N	LEU B 14	48 1	9.033	17.472	40.448	1.00	22.08	N
	MOTA	2081	CA	LEU B 14	48 1	.8.861	18.919	40.465	1.00	21.25	С
20	MOTA	2082	CB	LEU B 14	48 1	.9.545	19.556	39.255	1.00	22.23	С
	MOTA	2083	CG	LEU B 14	48 1	9.335	21.066	39.029	1.00	23.35	С
	MOTA	2084	CD1	LEU B 14	48 1	9.992	21.874	40.123	1.00	24.17	С
	MOTA	2085	CD2	LEU B 14	48 1	.9.920	21.453	37.696	1.00	25.57	С
	MOTA	2086	С	LEU B 14	48 1	7.383	19.275	40.467	1.00	20.22	С
25	MOTA	2087	0	LEU B 1	48 1	.6.664	18.997	39.510	1.00	19.83	0

	MOTA	2088	N	TYR B 149	16.937	19.865	41.567	1.00 20.43	N
	MOTA	2089	CA	TYR B 149	15.552	20.297	41.715	1.00 21.42	С
	ATOM	2090	СВ	TYR B 149	15.058	20.016	43.132	1.00 22.01	С
	MOTA	2091	CG	TYR B 149	14.633	18.591	43.344	1.00 23.22	С
5	ATOM	2092	CD1	TYR B 149	13.435	18.123	42.820	1.00 27.87	С
	ATOM	2093	CE1	TYR B 149	13.022	16.814	43.019	1.00 29.19	С
	ATOM	2094	CZ	TYR B 149	13.815	15.955	43.746	1.00 30.82	С
	ATOM	2095	OH	TYR B 149	13.394	14.659	43.937	1.00 37.77	0
	ATOM	2096	CE2	TYR B 149	15.020	16.390	44.277	1.00 30.92	С
10	ATOM	2097	CD2	TYR B 149	15.423	17.705	44.075	1.00 27.50	С
	MOTA	2098	С	TYR B 149	15.482	21.789	41.434	1.00 21.29	С
	ATOM	2099	0	TYR B 149	16.435	22.530	41.707	1.00 20.13	0
	ATOM	2100	N	SER B 150	14.350	22.223	40.895	1.00 21.81	N
	ATOM	2101	CA	SER B 150	14.144	23.623	40.557	1.00 22.08	С
15	ATOM	2102	CB	SER B 150	14.355	23.807	39.050	1.00 23.22	С
	ATOM	2103	OG	SER B 150	14.148	25.147	38.655	1.00 20.11	0
	MOTA	2104	С	SER B 150	12.745	24.116	40.946	1.00 22.46	С
	MOTA	2105	0	SER B 150	11.767	23.378	40.830	1.00 20.73	0
	ATOM	2106	N	ARG B 151	12.659	25.360	41.411	1.00 22.10	N
20	ATOM	2107	CA	ARG B 151	11.373	25.934	41.777	1.00 22.76	С
	MOTA	2108	СВ	ARG B 151	11.561	27.252	42.541	1.00 20.89	С
	MOTA	2109	CG	ARG B 151	12.009	27.087	43.994	1.00 19.59	С
	ATOM	2110	CD	ARG B 151	10.946	26.397	44.861	1.00 14.05	С
	MOTA	2111	NE	ARG B 151	11.344	26.371	46.270	1.00 16.55	N
25	ATOM	2112	CZ	ARG B 151	10.649	25.800	47.250	1.00 17.56	С

	MOTA	2113	NH1	ARG B	151	9.501	25.182	46.998	1.00 18.38	N
	MOTA	2114	NH2	ARG B	151	11.096	25.867	48.496	1.00 16.44	N
	MOTA	2115	С	ARG B	151	10.573	26.184	40.497	1.00 25.21	С
	MOTA	2116	0	ARG B	151	9.351	26.262	40.524	1.00 25.14	0
5	MOTA	2117	N _.	THR B	152	11.275	26.294	39.373	1.00 26.93	N
	MOTA	2118	CA	THR B	152	10.635	26.539	38.086	1.00 29.69	С
	MOTA	2119	СВ	THR B	152	11.167	27.824	37.451	1.00 29.18	С
	ATOM	2120	OG1	THR B	152	12.569	27.667	37.190	1.00 32.70	0
	ATOM	2121	CG2	THR B	152	10.956	29.007	38.377	1.00 30.82	С
10	ATOM	2122	С	THR B	152	10.922	25.403	37.116	1.00 31.23	С
	MOTA	2123	0	THR B	152	11.878	24.645	37.293	1.00 31.69	0
	ATOM	2124	N	GLN B	153	10.101	25.300	36.080	1.00 32.65	N
	MOTA	2125	CA	GLN B	153	10.283	24.264	35.077	1.00 35.10	С
	ATOM	2126	СВ	GLN B	153	8.985	24.043	34.322	1.00 35.06	С
15	ATOM	2127	CG	GLN B	153	7.878	23.553	35.214	1.00 36.53	С
	MOTA	2128	CD	GLN B	153	6.621	23.266	34.447	1.00 38.81	С
	MOTA	2129	OE1	GLN B	153	6.607	22.421	33.560	1.00 42.69	0
	MOTA	2130	NE2	GLN B	153	5.554	23.970	34.780	1.00 37.04	N
	MOTA	2131	С	GLN B	153	11.394	24.614	34.100	1.00 36.36	С
20	MOTA	2132	0	GLN B	153	11.876	23.755	33.368	1.00 37.01	0
	MOTA	2133	N	THR B	154	11.802	25.877	34.100	1.00 38.47	N
	MOTA	2134	CA	THR B	154	12.862	26.341	33.217	1.00 40.05	С
	MOTA	2135	СВ	THR B	154	12.584	27.772	32.722	1.00 40.61	С
	MOTA	2136	OG1	THR B	154	11.270	27.831	32:153	1.00 42.12	0
25	MOTA	2137	CG2	THR B	154	13.605	28.183	31.668	1.00 40.94	С

	ATOM	2138	С	THR B 154	14.169	26.333	33.992	1.00 40.87	С
	MOTA	2139	0	THR B 154	14.198	26.665	35.180	1.00 42.00	0
	MOTA	2140	N	LEU B 155	15.249	25.956	33.319	1.00 40.55	N
	MOTA	2141	CA	LEU B 155	16.554	25.888	33.961	1.00 41.78	С
5	MOTA	2142	СВ	LEU B 155	17.058	24.441	33.923	1.00 41.27	С
	ATOM	2143	CG	LEU B 155	17.825	23.880	35.120	1.00 41.78	С
	ATOM	2144	CD1	LEU B 155	16.977	23.974	36.390	1.00 36.65	С
	MOTA	2145	CD2	LEU B 155	18.186	22.432	34.828	1.00 40.61	С
	ATOM	2146	С	LEU B 155	17.556	26.810	33.266	1.00 42.44	С
10	ATOM	2147	0	LEU B 155	17.723	26.751	32.045	1.00 42.40	0
	ATOM	2148	N	LYS B 156	18.214	27.667	34.041	1.00 42.99	N
	ATOM	2149	CA	LYS B 156	19.206	28.580	33.485	1.00 43.59	С
	ATOM	2150	СВ	LYS B 156	19.458	29.743	34.449	1.00 43.63	С
	ATOM	2151	CG	LYS B 156	18.268	30.680	34.561	1.00 45.43	С
15	ATOM	2152	CD	LYS B 156	18.510	31.823	35.528	1.00 45.63	С
	ATOM	2153	CE	LYS B 156	17.297	32.749	35.567	1.00 47.26	С
	ATOM	2154	NZ	LYS B 156	17.407	33.814	36.609	1.00 47.89	N
	ATOM	2155	С	LYS B 156	20.509	27.836	33.203	1.00 43.26	С
	ATOM	2156	0	LYS B 156	20.967	27.032	34.012	1.00 41.69	0
20	ATOM	2157	N	ASP B 157	21.098	28.110	32.045	1.00 44.05	N
	MOTA	2158	CA	ASP B 157	22.340	27.463	31.637	1.00 44.05	С
	MOTA	2159	СВ	ASP B 157	22.901	28.163	30.402	1.00 45.56	С
	MOTA	2160	CG	ASP B 157	22.056	27.924	29.172	1.00 46.47	С
	MOTA	2161	OD1	ASP B 157	20.830	28.140	29.243	1.00 49.10	0
25	MOTA	2162	OD2	ASP B 157	22.619	27.521	28.134	1.00 50.45	0

	MOTA	2163	С	ASP B	157	23.403	27.410	32.732	1.00	43.87	С
	ATOM	2164	0	ASP B	157	24.088	26.396	32.891	1.00	43.50	0
	ATOM	2165	N	GLU B	158	23.548	28.492	33.487	1.00	43.29	N
	ATOM	2166	CA	GLU B	158	24.536	28.512	34.555	1.00	42.24	С
5	ATOM	2167	СВ	GLU B	158	24.580	29.895	35.211	1.00	43.13	С
	MOTA	2168	CG	GLU B	158	23.234	30.592	35.298	1.00	45.98	С
	MOTA	2169	CD	GLU B	158	23.329	32.071	34.947	1.00	48.36	С
	MOTA	2170	OE1	GLU B	158	24.183	32.773	35.533	1.00	48.34	0
	MOTA	2171	OE2	GLU B	158	22.545	32.529	34.085	1.00	49.65	0
10	MOTA	2172	С	GLU B	158	24.222	27.432	35.581	1.00	40.64	С
	ATOM	2173	0	GLU B	158	25.115	26.915	36.250	1.00	39.52	0
	MOTA	2174	N	LEU B	159	22.945	27.080	35.681	1.00	39.39	N
	MOTA	2175	CA	LEU B	159	22.494	26.051	36.613	1.00	37.85	С
	MOTA	2176	CB	LEU B	159	20.995	26.202	36.847	1.00	38.48	С
15	MOTA	2177	CG	LEU B	159	20.420	25.783	38.196	1.00	38.76	С
	ATOM	2178	CD1	LEU B	159	21.193	26.457	39.314	1.00	39.56	С
	ATOM	2179	CD2	LEU B	159	18.948	26.167	38.248	1.00	38.13	С
	ATOM	2180	С	LEU B	159	22.806	24.687	36.005	1.00	37.07	С
	ATOM	2181	0	LEU B	159	23.174	23.742	36.703	1.00	36.52	0
20	ATOM	2182	N	LYS B	160	22.661	24.591	34.690	1.00	36.16	N
	ATOM	2183	CA	LYS B	160	22.968	23.358	33.992	1.00	35.31	С
	MOTA	2184	СВ	LYS B	160	22.590	23.471	32.517	1.00	36.22	С
	ATOM	2185	CG	LYS B	160	21.096	23.433	32.231	1.00	37.33	С
	MOTA	2186	CD	LYS B	160	20.848	23.347	30.727	1.00	38.65	С
25	ATOM	2187	CE	LYS B	160	19.369	23.283	30.398	1.00	40.87	С

	MOTA	2188	NZ	LYS B	160	19.138	23.283	28.921	1.00	44.32	N
	MOTA	2189	С	LYS B	160	24.465	23.068	34.113	1.00	34.93	С
	MOTA	2190	0	LYS B	160	24.875	21.920	34.311	1.00	34.72	0
	ATOM	2191	N	GLU B	161	25.278	24.115	33.999	1.00	33.85	N
5	MOTA	2192	CA	GLU B	161	26.730	23.981	34.089	1.00	33.69	С
	MOTA	2193	СВ	GLU B	161	27.388	25.316	33.729	1.00	34.67	С
	MOTA	2194	CG	GLU B	161	27.208	25.686	32.260	1.00	36.90	С
	MOTA	2195	CD	GLU B	161	27.516	27.143	31.964	1.00	44.37	С
	MOTA	2196	OE1	GLU B	161	28.518	27.668	32.504	1.00	44.62	0
10	ATOM	2197	OE2	GLU B	161	26.759	27.761	31.179	1.00	45.41	0
	ATOM	2198	С	GLU B	161	27.163	23.522	35.478	1.00	32.63	С
	ATOM	2199	0	GLU B	161	28.034	22.658	35.623	1.00	32.33	0
	MOTA	2200	N	LYS B	162	26.542	24.088	36.503	1.00	32.15	N
	ATOM	2201	CA	LYS B	162	26.868	23.700	37.862	1.00	31.19	С
15	ATOM	2202	СВ	LYS B	162	26.037	24.515	38.858	1.00	32.11	С
	ATOM	2203	CG	LYS B	162	26.316	24.191	40.317	1.00	30.24	С
	ATOM	2204	CD	LYS B	162	25.256	24.803	41.226	1.00	29.84	С
	MOTA	2205	CE	LYS B	162	25.296	26.322	41.201	1.00	28.84	С
	ATOM	2206	NZ	LYS B	162	26.579	26.847	41.743	1.00	28.90	N
20	ATOM	2207	С	LYS B	162	26.595	22.209	38.044	1.00	29.86	С
	MOTA	2208	0	LYS B	162	27.412	21.490	38.612	1.00	30.46	0
	MOTA	2209	N	PHE B	163	25.450	21.751	37.546	1.00	29.69	N
	MOTA	2210	CA	PHE B	163	25.054	20.346	37.655	1.00	29.00	С
	MOTA	2211	СВ	PHE B	163	23.648	20.157	37.071	1.00	28.39	С
25	MOTA	2212	CG	PHE B	163	23.074	18.795	37.301	1.00	26.32	С

	MOTA	2213	CD1	PHE B 16	3 22.834	18.337	38.587	1.00 22.99	С
	ATOM	2214	CE1	PHE B 16	3 22.304	17.077	38.802	1.00 22.53	С
	MOTA	2215	CZ	PHE B 16	3 22.007	16.256	37.723	1.00 21.90	С
	MOTA	2216	CE2	PHE B 16	3 22.239	16.698	36.440	1.00 25.70	С
5	MOTA	2217	CD2	PHE B 16	3 22.771	17.963	36.231	1.00 26.75	С
	MOTA	2218	С	PHE B 16	3 26.038	19.432	36.933	1.00 29.29	С
	MOTA	2219	0	PHE B 16	3 26.504	18.434	37.487	1.00 30.36	0
	MOTA	2220	N	THR B 16	4 26.348	19.772	35.688	1.00 30.76	N
	MOTA	2221	CA	THR B 16	4 27.291	18.981	34.904	1.00 31.26	С
10	MOTA	2222	CB	THR B 16	4 27.446	19.556	33.478	1.00 30.79	С
	MOTA	2223	OG1	THR B 16	4 26.173	19.540	32.817	1.00 32.00	0
	MOTA	2224	CG2	THR B 16	4 28.432	18.716	32.664	1.00 33.63	С
	MOTA	2225	С	THR B 16	4 28.657	18.958	35.595	1.00 30.45	С
	MOTA	2226	0	THR B 16	4 29.313	17.915	35.660	1.00 31.24	0
15	MOTA	2227	N	THR B 16	5 29.079	20.107	36.114	1.00 30.54	N
	MOTA	2228	CA	THR B 16	5 30.359	20.202	36.811	1.00 31.33	С
	MOTA	2229	СВ	THR B 16	5 30.640	21.648	37.243	1.00 31.71	С
	MOTA	2230	OG1	THR B 16	5 30.720	22.475	36.078	1.00 32.17	0
	MOTA	2231	CG2	THR B 16	5 31.945	21.738	38.013	1.00 31.92	С
20	MOTA	2232	С	THR B 16	5 30.385	19.305	38.050	1.00 31.31	С
	MOTA	2233	0	THR B 16	5 31.304	18.499	38.228	1.00 30.04	0
	MOTA	2234	N	PHE B 16	6 29.378	19.451	38.908	1.00 31.86	N
	MOTA	2235	CA	PHE B 16	6 29.300	18.635	40.111	1.00 32.35	С
	MOTA	2236	СВ	PHE B 16	6 28.069	19.007	40.939	1.00 31.30	С
25	ATOM	2237	CG	PHE B 16	6 27.861	18.121	42.138	1.00 34.42	С

	MOTA	2238	CD1	PHE B 1	.66	28.755	18.149	43.206	1.00	32.31	С
	MOTA	2239	CE1	рне в 1	.66	28.580	17.302	44.303	1.00	28.62	С
	MOTA	2240	CZ	рне в 1	.66	27.505	16.420	44.337	1.00	29.27	С
	MOTA	2241	CE2	рне в 1	.66	26.610	16.386	43.281	1.00	34.35	С
5	MOTA	2242	CD2	рне в 1	.66	26.790	17.234	42.187	1.00	33.74	С
	MOTA	2243	С	рне в 1	.66	29.224	17.153	39.739	1.00	32.79	С
	MOTA	2244	0	PHE B 1	.66	29.836	16.304	40.398	1.00	34.11	0
	MOTA	2245	N	SER B 1	.67	28.471	16.847	38.687	1.00	33.75	N
	MOTA	2246	CA	SER B 1	.67	28.311	15.464	38.245	1.00	33.72	С
10	ATOM	2247	СВ	SER B 1	.67	27.298	15.385	37.102	1.00	32.77	С
	ATOM	2248	OG	SER B 1	.67	26.006	15.736	37.551	1.00	32.40	0
	MOTA	2249	С	SER B 1	.67	29.629	14.854	37.791	1.00	34.67	С
	MOTA	2250	0	SER B 1	.67	29.936	13.701	38.102	1.00	34.94	0
	MOTA	2251	N	LYS B 1	.68	30.404	15.630	37.048	1.00	35.59	N
15	MOTA	2252	CA	LYS B 1	.68	31.679	15.145	36.555	1.00	36.93	Ċ
	MOTA	2253	СВ	LYS B 1	.68	32.221	16.099	35.488	1.00	37.02	С
	MOTA	2254	CG	LYS B 1	.68	31.407	16.084	34.194	1.00	38.92	С
	MOTA	2255	CD	LYS B 1	.68	31.949	17.072	33.171	1.00	39.84	С
	MOTA	2256	CE	LYS B 1	.68	31.218	16.942	31.845	1.00	42.88	С
20	MOTA	2257	NZ	LYS B 1	.68	31.693	17.934	30.832	1.00	42.91	N
	MOTA	2258	С	LYS B 1	.68	32.658	15.002	37.713	1.00	37.30	С
	MOTA	2259	0	LYS B 1	.68	33.441	14.053	37.758	1.00	36.54	0
	MOTA	2260	N	ALA B 1	.69	32.589	15.934	38.661	1.00	38.00	N
	MOTA	2261	CA	ALA B 1	.69	33.460	15.906	39.828	1.00	38.86	С
25	MOTA	2262	СВ	ALA B 1	.69	33.263	17.165	40.655	1.00	37.89	С

	MOTA	2263	С	ALA B	169	33.171	14.670	40.671	1.00	39.70	С
	ATOM	2264	0	ALA B	169	33.854	14.408	41.660	1.00	41.32	0
	ATOM	2265	N	GLN B	170	32.157	13.910	40.275	1.00	40.38	N
	MOTA	2266	CA	GLN B	170	31.785	12.696	40.992	1.00	39.99	С
5	ATOM	2267	СВ	GLN B	170	30.317	12.763	41.415	1.00	39.42	С
	MOTA	2268	CG	GLN B	170	30.049	13.757	42.528	1.00	36.89	С
	MOTA	2269	CD	GLN B	170	30.870	13.469	43.770	1.00	37.17	С
	MOTA	2270	OE1	GLN B	170	30.931	12.327	44.235	1.00	36.89	0
	MOTA	2271	NE2	GLN B	170	31.502	14.501	44.317	1.00	33.10	N
10	MOTA	2272	С	GLN B	170	32.019	11.456	40.137	1.00	40.67	С
	MOTA	2273	0	GLN B	170	31.554	10.361	40.464	1.00	40.53	0
	MOTA	2274	N	GLY B	171	32.739	11.637	39.034	1.00	42.18	N
	MOTA	2275	CA	GLY B	171	33.031	10.519	38.158	1.00	42.99	С
	MOTA	2276	С	GLY B	171	31.891	10.138	37.234	1.00	44.08	С
15	MOTA	2277	0	GLY B	171	31.738	8.970	36.870	1.00	44.03	0
	MOTA	2278	N	LEU B	172	31.077	11.118	36.861	1.00	44.44	N
	MOTA	2279	CA	LEU B	172	29.966	10.863	35.957	1.00	44.81	С
	MOTA	2280	СВ	LEU B	172	28.664	11.432	36.524	1.00	45.23	С
	MOTA	2281	CG	LEU B	172	28.158	10.879	37.858	1.00	44.93	С
20	MOTA	2282	CD1	LEU B	172	26.829	11.536	38.188	1.00	45.43	С
	MOTA	2283	CD2	LEU B	172	27.993	9.368	37.783	1.00	45.17	С
	ATOM	2284	С	LEU B	172	30.281	11.524	34.624	1.00	45.45	С
	ATOM	2285	0	LEU B	172	30.717	12.675	34.576	1.00	45.61	0
	MOTA	2286	N	THR B	173	30.073	10.788	33.541	1.00	45.63	N
25	ATOM	2287	CA	THR B	173	30.338	11.309	32.209	1.00	46.03	С

	MOTA	2288	CB	THR B	173	30.765	10.183	31.267	1.00	45.95	С
	MOTA	2289	OG1	THR B	173	29.743	9.183	31.228	1.00	47.13	0
	ATOM	2290	CG2	THR B	173	32.054	9.545	31.761	1.00	46.88	С
	ATOM	2291	С	THR B	173	29.089	11.981	31.651	1.00	45.65	С
5	ATOM	2292	0	THR B	173	27.991	11.801	32.179	1.00	45.14	0
	ATOM	2293	N	GLU B	174	29.260	12.751	30.581	1.00	45.76	N
	ATOM	2294	CA	GLU B	174	28.140	13.448	29.969	1.00	45.79	С
	MOTA	2295	СВ	GLU B	174	28.615	14.278	28.777	1.00	46.84	С
	ATOM	2296	CG	GLU B	174	29.518	15.428	29.181	1.00	49.10	С
10	ATOM	2297	CD	GLU B	174	29.375	16.630	28.273	1.00	51.93	С
	ATOM	2298	OE1	GLU B	174	29.639	16.496	27.058	1.00	53.25	0
	ATOM	2299	OE2	GLU B	174	28.993	17.709	28.775	1.00	50.59	0
	ATOM	2300	С	GLU B	174	27.032	12.501	29.541	1.00	44.90	С
	ATOM	2301	0	GLU B	174	25.850	12.846	29.615	1.00	45.22	0
15	ATOM	2302	N	GLU B	175	27.401	11.304	29.100	1.00	43.45	N
	ATOM	2303	CA	GLU B	175	26.389	10.341	28.693	1.00	42.73	С
	ATOM	2304	CB	GLU B	175	27.028	9.121	28.017	1.00	43.30	С
	MOTA	2305	CG	GLU B	175	28.093	8.403	28.815	1.00	47.17	С
	ATOM	2306	CD	GLU B	175	27.817	6.913	28.917	1.00	52.72	С
20	ATOM	2307	OE1	GLU B	175	27.495	6.295	27.877	1.00	54.49	0
	MOTA	2308	OE2	GLU B	175	27.922	6.359	30.034	1.00	54.58	0
	MOTA	2309	С	GLU B	175	25.582	9.918	29.916	1.00	40.71	С
•	MOTA	2310	0	GLU B	175	24.478	9.390	29.793	1.00	40.87	0
	MOTA	2311	N	ASP B	176	26.136	10.166	31.099	1.00	39.09	N
25	ATOM	2312	CA	ASP B	176	25.460	9.826	32.345	1.00	38.13	С

	MOTA	2313	CB	ASP B 17	76 26.465	9.332	33.391	1.00 38.20	С
	MOTA	2314	CG	ASP B 17	26.930	7.910	33.132	1.00 38.78	С
	MOTA	2315	OD1	ASP B 17	26.083	7.055	32.782	1.00 36.70	0
	MOTA	2316	OD2	ASP B 17	76 28.139	7.644	33.296	1.00 40.22	0
5	MOTA	2317	С	ASP B 17	76 24.693	11.019	32.912	1.00 36.59	С
	MOTA	2318	0	ASP B 17	76 24.104	10.930	33.982	1.00 36.42	0
	MOTA	2319	'n	ILE B 17	77 24.698	12.130	32.191	1.00 35.68	N
	MOTA	2320	CA	ILE B 17	77 24.017	13.332	32.650	1.00 34.90	С
	MOTA	2321	СВ	ILE B 17	25.009	14.507	32.722	1.00 35.58	С
10	ATOM	2322	CG1	ILE B 17	77 26.172	14.132	33.649	1.00 33.32	С
	MOTA	2323	CD1	ILE B 17	27.339	15.103	33.605	1.00 34.46	С
	MOTA	2324	CG2	ILE B 17	77 24.301	15.762	33.207	1.00 34.43	С
	MOTA	2325	С	ILE B 17	22.855	13.697	31.729	1.00 34.02	C
	MOTA	2326	0	ILE B 17	23.002	13.704	30.509	1.00 33.69	0
15	MOTA	2327	N .	VAL B 17	28 21.701	13.996	32.316	1.00 32.85	N
	MOTA	2328	CA	VAL B 17	78 20.532	14.345	31.517	1.00 31.32	С
	MOTA	2329	СВ	VAL B 17	78 19.650	13.107	31.252	1.00 31.12	С
	MOTA	2330	CG1	VAL B 17	78 19.180	12.513	32.563	1.00 31.16	С
	ATOM	2331	CG2	VAL B 17	8 18.445	13.500	30.400	1.00 33.20	С
20	MOTA	2332	С	VAL B 17	19.637	15.412	32.122	1.00 29.38	С
	MOTA	2333	0	VAL B 17	78 19.302	15.355	33.295	1.00 30.40	0
	MOTA	2334	N	PHE B 17	79 _. 19.248	16.387	31.308	1.00 28.78	N
	MOTA	2335	CA	PHE B 17	79 18.341	17.438	31.759	1.00 28.53	С
	MOTA	2336	СВ	PHE B 17	79 18.737	18.786	31.143	1.00 27.73	С
25	MOTA	2337	CG	PHE B 17	9 20.042	19.315	31.684	1.00 29.80	С

	MOTA	2338	CD1	PHE B	179	20.116	19.813	32.983	1.00 30.84	С
	MOTA	2339	CE1	PHE B	179	21.336	20.190	33.544	1.00 32.23	С
	MOTA	2340	CZ	PHE B	179	22.502	20.072	32.797	1.00 34.74	С
	MOTA	2341	CE2	PHE B	179	22.443	19.582	31.492	1.00 33.64	С
5	MOTA	2342	CD2	PHE B	179	21.215	19.209	30.942	1.00 32.32	С
	MOTA	2343	С	PHE B	179	16.956	16.974	31.331	1.00 29.31	С
	MOTA	2344	0	PHE B	179	16.622	16.949	30.143	1.00 29.18	0
	MOTA	2345	N	LEU B	180	16.178	16.565	32.330	1.00 30.16	N
	ATOM	2346	CA	LEU B	180	14.836	16.031	32.150	1.00 29.93	С
10	MOTA	2347	СВ	LEU B	180	14.245	15.708	33.524	1.00 30.00	С
	MOTA	2348	CG	LEU B	180	15.155	14.806	34.375	1.00 30.73	С
	ATOM	2349	CD1	LEU B	180	14.558	14.593	35.762	1.00 26.95	С
	ATOM	2350	CD2	LEU B	180	15.352	13.468	33.672	1.00 26.54	С
	MOTA	2351	С	LEU B	180	13.887	16.912	31.351	1.00 30.61	С
15	ATOM	2352	0	LEU B	180	13.620	18.057	31.720	1.00 30.66	0
	MOTA	2353	N	PRO B	181	13.362	16.382	30.232	1.00 32.29	N
	MOTA	2354	CA	PRO B	181	12.437	17.139	29.388	1.00 33.25	С
	MOTA	2355	CB	PRO B	181	12.331	16.276	28.134	1.00 33.09	С
	MOTA	2356	CG	PRO B	181	12.459	14.902	28.676	1.00 33.42	С
20	MOTA	2357	CD	PRO B	181	13.589	15.036	29.674	1.00 30.91	С
	MOTA	2358	С	PRO B	181	11.091	17.341	30.070	1.00 34.85	С
	MOTA	2359	0	PRO B	181	10.603	16.463	30.773	1.00 33.36	0
	MOTA	2360	N	GLN B	182	10.509	18.517	29.853	1.00 37.61	N
	MOTA	2361	CA	GLN B	182	9.220	18.878	30.421	1.00 41.17	С
25	MOTA	2362	СВ	GLN B	182	8.963	20.365	30.174	1.00 41.43	С

	MOTA	2363	CG	GLN B	182	7.645	20.876	30.706	1.00 43.3	12	С
	ATOM	2364	CD	GLN B	182	7.403	22.321	30.326	1.00 46.6	58	С
	ATOM	2365	OE1	GLN B	182	8.151	23.214	30.729	1.00 45.8	35	0
	ATOM	2366	NE2	GLN B	182	6.360	22.559	29.536	1.00 46.6	54	N
5	ATOM	2367	С	GLN B	182	8.095	18.043	29.805	1.00 42.8	35	С
	ATOM	2368	0	GLN B	182	7.862	18.090	28.602	1.00 43.9	90	0
	ATOM	2369	N	PRO B	183	7.390	17.257	30.629	1.00 44.6	53	N
	MOTA	2370	CA	PRO B	183	6.288	16.416	30.150	1.00 46.1	L7	С
	MOTA	2371	СВ	PRO B	183	5.904	15.610	31.390	1.00 45.6	50	С
10	MOTA	2372	CG	PRO B	183	7.167	15.564	32.173	1.00 45.8	32	С
	ATOM	2373	CD	PRO B	183	7.687	16.964	32.038	1.00 44.4	10	С
	MOTA	2374	С	PRO B	183	5.130	17.272	29.657	1.00 47.4	17	С
	MOTA	2375	0	PRO B	183	4.973	18.413	30.091	1.00 47.6	56	0
	MOTA	2376	N	ASP B	184	4.319	16.726	28.757	1.00 49.5	52	N
15	MOTA	2377	CA	ASP B	184	3.181	17.470	28.239	1.00 52.2	24	С
	MOTA	2378	СВ	ASP B	184	2.737	16.898	26.891	1.00 52.8	39	С
	ATOM	2379	CG	ASP B	184	2.513	17.982	25.849	1.00 55.9	95	С
	ATOM	2380	OD1	ASP B	184	3.480	18.715	25.534	1.00 57.8	37	0
	ATOM	2381	OD2	ASP B	184	1.373	18.107	25.346	1.00 61.1	13	0
20	ATOM	2382	С	ASP B	184	2.034	17.410	29.248	1.00 53.0	04	С
	ATOM	2383	0	ASP B	184	1.228	18.332	29.343	1.00 53.2	26	0
	ATOM	2384 .	N	LYS B	185	1.975	16.321	30.007	1.00 54.2	24	N
	ATOM	2385	CA	LYS B	185	0.945	16.148	31.024	1.00 55.5	51	С
	ATOM	2386	СВ	LYS B	185	-0.080	15.100	30.578	1.00 55	.50	С
25	ATOM	2387	CG	LYS B	185	0.500	13.738	30.233	1.00 57.3	16	С

	MOTA	2388	CD	LYS B	185	-0.576	12.827	29.658	1.00 59.05	С
	ATOM	2389	CE	LYS B	185	0.029	11.582	29.027	1.00 60.15	С
	ATOM	2390	NZ	LYS B	185	-0.982	10.804	28.253	1.00 62.13	N
	MOTA	2391	С	LYS B	185	1.569	15.728	32.351	1.00 55.95	С
5	MOTA	2392	0	LYS B	185	2.792	15.651	32.472	1.00 55.12	0
	MOTA	2393	N	CYS B	186	0.716	15.473	33.340	1.00 57.05	N
	MOTA	2394	CA	CYS B	186	1.139	15.050	34.675	1.00 58.53	С
	MOTA	2395	СВ	CYS B	186	2.096	13.857	34.595	1.00 57.56	C
	MOTA	2396	SG	CYS B	186	1.530	12.467	33.576	1.00 54.12	S
10	MOTA	2397	С	CYS B	186	1.815	16.131	35.513	1.00 60.82	С
	MOTA	2398	0	CYS B	186	2.384	15.823	36.559	1.00 61.78	0
	MOTA	2399	N	ILE B	187	1.763	17.387	35.080	1.00 63.56	N
	MOTA	2400	CA	ILE B	187	2.415	18.454	35.839	1.00 66.53	С
	MOTA	2401	СВ	ILE B	187	3.874	18.652	35.363	1.00 66.78	С
15	MOTA	2402	CG1	ILE B	187	4.702	17.408	35.696	1.00 66.73	С
	MOTA	2403	CD1	ILE B	187	6.159	17.512	35.298	1.00 69.46	С
	MOTA	2404	CG2	ILE B	187	4.487	19.879	36.026	1.00 67.81	С
	MOTA	2405	С	ILE B	187	1.711	19.806	35.806	1.00 68.53	С
	MOTA	2406	0	ILE B	187	1.952	20.651	36.669	1.00 69.20	0
20	ATOM	2407	N	GLN B	188	0.855	20.003	34.805	1.00 71.16	N
	MOTA	2408	CA	GLN B	188	0.093	21.243	34.635	1.00 73.58	С
	MOTA	2409	СВ	GLN B	188	-0.529	21.695	35.961	1.00 73.62	С
	ATOM	2410	CG	GLN B	188	-1.130	20.595	36.807	1.00 75.18	С
	ATOM	2411	CD	GLN B	188	-1.452	21.083	38.206	1.00 78.27	С
25	ATOM	2412	OE1	GLN E	188	-0.749	21.937	38.748	1.00 79.42	0

	MOTA	2413	NE2	GLN	В	188	-2.502	20.535	38.806	1.00 78.56	N
	MOTA	2414	С	GLN	В	188	0.950	22.385	34.095	1.00 75.04	С
	MOTA	2415	О	GLN	В	188	0.985	23.464	34.687	1.00 75.36	0
	MOTA	2416	N	GLU	В	189	1.628	22.136	32.977	1.00 76.95	N
5	MOTA	2417	CA	GLU	В	189	2.494	23.116	32.311	1.00 78.69	С
	MOTA	2418	CB	GLU	В	189	3.166	24.058	33.320	1.00 79.07	С
	MOTA	2419	CG	GLU	В	189	2.460	25.402	33.534	1.00 81.42	С
	MOTA	2420	CD	GLU	В	189	2.511	26.310	32.312	1.00 84.40	С
	MOTA	2421	OE1	GLU	В	189	1.987	25.916	31.246	1.00 85.84	0
10	MOTA	2422	OE2	GLU	В	189	3.073	27.423	32.419	1.00 84.76	0
	MOTA	2423	С	GLU	В	189	3.572	22.399	31.504	1.00 79.10	С
	MOTA	2424	0	GLU	В	189	4.766	22.599	31.810	1.00 79.70	0
	MOTA	2425	OXT	GLU	В	189	3.209	21.644	30.576	1.00 79.48	0
	MOTA	2426	0	НОН	W	1	4.040	12.508	8.261	1.00 26.70	0
15	MOTA	2427	0	нон	W	2	13.933	21.047	-5.444	1.00 32.16	0
	MOTA	2428	0	НОН	W	3	14.595	10.712	-6.463	1.00 26.68	0
	MOTA	2429	0	НОН	W	4	19.496	15.770	2.484	1.00 31.13	0
	MOTA	2430	0	НОН	W	5	18.407	11.181	-4.230	1.00 34.02	0
	MOTA	2431	0	нон	W	6	16.852	13.205	18.050	1.00 33.11	0
20	MOTA	2432	0	НОН	W	7	10.214	21.072	58.242	1.00 37.47	0
	MOTA	2433	0	нон	W	8	9.748	10.525	59.061	1.00 34.17	0
	MOTA	2434	0	НОН	W	9	20.458	12.571	44.330	1.00 35.78	0
	MOTA	2435	0	НОН	W	10	8.700	11.028	45.277	1.00 51.91	0
	MOTA	2436	0	НОН	W	11	16.314	26.308	10.121	1.00 33.23	0
25	MOTA	2437	0	НОН	W	12	15.210	20.001	32.653	1.00 39.92	0

	MOTA	2438	0	HOH W	13	3.960	5.716	47.160	1.00 45.80	0
	MOTA	2439	0	HOH W	14	26.435	17.047	49.748	1.00 40.15	0
	MOTA	2440	0	HOH W	15	-1.112	11.755	2.219	1.00 64.01	0
	MOTA	2441	0	HOH W	16	10.171	28.451	50.750	1.00 43.61	0
5	MOTA	2442	0	HOH W	17	10.104	20.203	4.975	1.00 53.19	0
	MOTA	2443	0	HOH W	18	20.745	16.542	-2.769	1.00 28.77	0
	MOTA	2444	0	HOH W	19	-5.660	-7.610	5.960	1.00 45.24	0
	MOTA	2445	0	HOH W	20	9.000	20.045	19.857	1.00 38.22	0
	MOTA	2446	0	HOH W	21	8.480	7.462	30.871	1.00 47.46	0
10	MOTA	2447	0	HOH W	22	27.822	17.883	54.991	1.00 28.92	0
	MOTA	2448	0	HOH W	23	2.188	18.872	32.043	1.00 48.84	0
	MOTA	2449	0	HOH W	24	17.633	18.838	57.504	1.00 41.89	0
	MOTA	2450	0	HOH W	25	21.652	25.017	51.935	1.00 57.47	0
	MOTA	2451	0	HOH W	26	7.604	12.850	34.861	1.00 41.07	0
15	MOTA	2452	0	HOH W	27	25.207	11.648	50.638	1.00 69.60	0
	MOTA	2453	0	HOH W	29	16.729	13.179	27.696	1.00 47.29	0
	MOTA	2454	0	HOH W	30	5.081	13.816	26.987	1.00 66.72	0
	MOTA	2455	0	HOH W	31	12.960	30.863	40.957	1.00 47.76	0
	MOTA	2456	0	HOH W	32	15.970	11.521	7.301	1.00 49.79	0
20	MOTA	2457	0	HOH W	33	21.271	23.315	14.636	1.00 42.32	0
	MOTA	2458	0	HOH W	34	5.009	10.689	25.767	1.00 58.86	0
	MOTA	2459	0	HOH W	35	1.694	10.843	-1.667	1.00 38.92	0
	MOTA	2460	0	HOH W	36	-0.310	25.857	2.103	1.00 60.86	0
	MOTA	2461	0	HOH W	37	-8.796	15.352	6.606	1.00 69.93	0
25	ATOM	2462	0	HOH W	38	20.951	15.510	-0.080	1.00 28.14	0

	MOTA	2463	0	HOH W	39	15.352	11.784	30.109	1.00 51.67	0
	MOTA	2464	0	нон w	40	3.355	14.719	53.024	1.00 37.70	0
	MOTA	2465	0	HOH W	42	-2.050	9.295	-4.545	1.00 57.33	0
	MOTA	2466	0	HOH W	43	-9.976	9.916	9.991	1.00 87.82	0
5	MOTA	2467	0	HOH W	44	5.572	21.524	-2.004	1.00 74.94	0
	MOTA	2468	0 ,	HOH W	46	9.193	11.834	22.390	1.00 50.58	Ō
	MOTA	2469	0	W HOH	47	17.876	15.823	58.201	1.00 45.45	0
	MOTA	2470	0	нон и	48	10.186	1.800	11.898	1.00 58.91	0
	MOTA	2471	0	HOH W	49	9.488	10.004	34.123	1.00 48.87	0
10	MOTA	2472	0	HOH W	50	0.567	26.733	39.027	1.00 52.93	0
	MOTA	2473	0	HOH W	51	10.518	24.208	-7.159	1.00 43.91	0
	MOTA	2474	0	HOH W	52	11.275	31.220	11.609	1.00 72.49	0
	MOTA	2475	0	HOH W	53	20.256	5.993	5.735	1.00 48.72	0
	MOTA	2476	0	HOH W	54	-4.488	19.914	37.431	1.00 55.84	0
15	MOTA	2477	0	W HOH	55	9.259	18.064	3.239	1.00 58.33	0
	MOTA	2478	0	HOH W	56	23.933	22.944	51.722	1.00 54.99	0
	MOTA	2479	0	HOH W	57	24.841	9.119	-0.096	1.00 53.03	0
	MOTA	2480	0	HOH W	58	4.424	16.540	23.959	1.00 45.30	0
	MOTA	2481	0	HOH W	59	23.572	18.774	53.301	1.00 43.19	0
20	MOTA	2482	0	HOH W	60	19.627	11.112	27.097	1.00 56.82	0
	MOTA	2483	0	HOH W	61	7.728	25.890	42.676	1.00 40.99	0
	MOTA	2484	0	HOH W	62	13.333	1.796	4.471	1.00 48.50	0
	MOTA	2485	0	HOH W	63	5.991	15.776	-5.712	1.00 36.49	0
	MOTA	2486	0	HOH W	65	6.100	10.580	56.983	1.00 44.25	0
25	ATOM	2487	0	HOH W	66	10.175	17.800	-9.148	1.00 50.73	0

	MOTA	2488	0	HOH W	67	12.429	10.671	26.357	1.00 43.62	0
	MOTA	2489	0	HOH W	68	14.092	19.997	47.805	1.00 56.02	0
	MOTA	2490	0	HOH W	69	27.526	13.816	40.679	1.00143.11	0
	MOTA	2491	0	HOH W	70	27.171	25.976	50.883	1.00 70.04	0
5	MOTA	2492	0	HOH W	71	25.949	13.041	12.265	1.00 61.46	0
	MOTA	2493	0	HOH W	73	20.947	34.715	46.208	1.00 68.24	0
	MOTA	2494	0	HOH W	74	16.555	26.377	22.214	1.00 59.16	0
	MOTA	2495	0	HOH W	75	-3.547	26.746	2.866	1.00 71.13	0
	ATOM	2496	0	HOH W	76	5.540	14.794	-9.696	1.00 69.89	0
10	ATOM	2497	0	HOH W	77	23.279	-0.635	39.750	1.00 62.15	0
	MOTA	2498	0	HOH W	80	19.922	16.795	28.541	1.00 44.27	0
	MOTA	2499	0	HOH W	81	27.483	11.963	53.993	1.00 45.20	0
	MOTA	2500	0	HOH W	82	13.906	22.578	32.044	1.00 55.11	0
	MOTA	2501	0	HOH W	83	22.987	24.494	12.307	1.00 58.59	0
15	ATOM	2502	0	HOH W	84	16.335	8.026	21.642	1.00 46.23	0
	MOTA	2503	0	HOH W	85	12.684	3.455	13.075	1.00 78.38	0
	MOTA	2504	0	HOH W	86	20.879	16.549	9.771	1.00 42.57	0
	MOTA	2505	0	HOH W	87	0.757	21.593	28.527	1.00 69.69	О
	MOTA	2506	0	HOH W	88	13.879	17.013	47.543	1.00 54.48	0
20	MOTA	2507	0	HOH W	89	15.694	18.445	49.669	1:00 54.79	0
	MOTA	2508	0	HOH W	90	-2.076	0.968	51.836	1.00 59.41	0
	MOTA	2509	0	HOH W	91	19.272	30.879	50.117	1.00 58.03	0
	MOTA	2510	0	HOH W	92	17.785	26.541	5.860	1.00 58.78	0
	ATOM	2511	0	HOH W	93	15.194	10.406	18.655	1.00 51.55	0
25	MOTA	2512	0	HOH W	94	14.191	10.352	15.784	1.00 59.53	0

	MOTA	2513	0	HOH W	95	14.530	8.322	12.335	1.00 57.57	0
	MOTA	2514	0	HOH W	96	14.382	6.550	1.265	1.00 39.82	0
	MOTA	2515	0	HOH W	97	3.491	9.628	-10.219	1.00 64.18	0
	ATOM	2516	0	HOH W	98	7.943	11.032	6.651	1.00 61.55	0
5	MOTA	2517	0	HOH W	99	2.917	34.621	6.036	1.00 76.28	0
	MOTA	2518	0	HOH W	100	6.976	33.080	4.434	1.00 63.23	0
	MOTA	2519	0	HOH W	101	4.575	31.407	2.694	1.00 62.67	0
	MOTA	2520	0	нон w	102	10.274	34.137	10.082	1.00 56.85	0
	ATOM	2521	0	HOH W	103	10.163	22.575	20.912	1.00 54.58	0
10	MOTA	2522	О	HOH W	104	8.270	24.585	21.965	1.00 47.21	0
	MOTA	2523	0	HOH W	105	17.520	21.811	53.118	1.00 56.66	0
	MOTA	2524	0	HOH W	106	9.883	6.038	51.329	1.00 35.50	0
	MOTA	2525	0	HOH W	107	14.590	8.397	41.921	1.00 81.43	0
	MOTA	2526	0	HOH W	108	16.218	11.381	46.157	1.00 72.99	0
15	MOTA	2527	0	HOH W	109	24.706	15.452	29.112	1.00 57.26	0
	MOTA	2528	0	HOH W	110	18.692	22.125	55.822	1.00 70.38	0
	MOTA	2529	0	HOH W	111	22.284	24.536	58.178	1.00 54.74	0
	MOTA	2530	0	HOH W	112	17.887	1.620	25.979	1.00 51.74	0
	MOTA	2531	0	HOH W	113	25.868	4.467	51.867	1.00 74.64	0

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Table 3

Three Dimensional Coordinates of Se-Met-type L-PGDS

ATOM 1 CB PHE A 34 -8.574 -24.037 55.181 1.00 80.07 A

ATOM 2 CG PHE A 34 -7.718 -22.864 54.718 1.00 79.58 A

25 ATOM 3 CD1 PHE A 34 -7.455 -22.691 53.358 1.00 78.93 A

	ATOM	4	CD2 1	PHE A	34	-7.119 -21.988	55.626	1.00 78.38	A
	MOTA	5	CE1	PHE A	34	-6.605 -21.683	52.908	1.00 77.67	A
	ATOM	6	CE2 1	PHE A	34	-6.265 -20.975	55.184	1.00 78.08	A
	MOTA	7	CZ I	PHE A	34	-6.008 -20.827	53.819	1.00 78.70	A
5	MOTA	8	C I	PHE A	34	-7.194 -24.354	57.289	1.00 78.35	A
	MOTA	9	O 1	PHE A	34	-6.887 -23.715	58.301	1.00 79.55	A
	ATOM	10	N	PHE A	34	-9.359 -23.145	57.369	1.00 80.95	A
	ATOM	11	CA	PHE A	34	-8.607 -24.254	56.712	1.00 79.32	A
	MOTA	12	N	GLN A	35	-6.335 -25.151	56.657	1.00 75.88	A
10	MOTA	13	CA	GLN A	35	-4.962 -25.309	57.136	1.00 72.38	A
	MOTA	14	CB	GLN A	35	-4.643 -26.790	57.280	1.00 74.51	A
	MOTA	15	CG	GLN A	35	-5.890 -27.647	57.401	1.00 75.90	A
	MOTA	16	CD	GLN A	35	-5.570 -29.094	57.698	1.00 76.72	Α.
	ATOM	17	OE1	GLN A	35	-5.107 -29.428	58.794	1.00 78.20	A
15	MOTA	18	NE2	GLN A	35	-5.808 -29.965	56.722	1.00 75.23	A
	ATOM .	19	С	GLN A	35	-4.008 -24.658	56.138	1.00 67.48	Α
	ATOM	20	0	GLN A	35	-3.528 -25.318	55.216	1.00 65.63	A
	MOTA	21	N	GLN A	36	-3.727 -23.369	56.335	1.00 62.20	A
	MOTA	22	CA	GLN A	36	-2.859 -22.638	55.420	1.00 55.74	A
20	ATOM	23	СВ	GLN A	36	-2.796 -21.139	55.794	1.00 53.90	A
	ATOM	24	CG	GLN A	36	-2.278 -20.778	57.183	1.00 53.70	Α
	ATOM	25	æ	GLN A	36	-1.986 -19.277	57.323	1.00 51.50	Α
	MOTA	26	OE1	GLN A	36	-2.866 -18.437	57.155	1.00 52.05	Α
	MOTA	27	NE2	GLN A	36	-0.742 -18.945	57.626	1.00 53.40	A
25	MOTA	28	С	GLN A	36	-1.453 -23.210	55.233	1.00 52.02	Α

	MOTA	29	0	GLN A	36	-0.789 -22.879	54.252	1.00 52.24	A
	MOTA	30	N	ASP A	37	-1.005 -24.066	56.155	1.00 49.11	A
	MOTA	31	CA	ASP A	37	0.317 -24.702	56.046	1.00 44.61	A
	MOTA	32	СВ	ASP A	37	0.564 -25.655	57.224	1.00 49.16	A
5	ATOM	33	CG	ASP A	37	1.188 -24.968	58.439	1.00 54.29	A
	MOTA	34	OD1	ASP A	37	2.411 -24.701	58.416	1.00 56.85	A
	MOTA	35	OD2	ASP A	37	0.461 -24.703	59.425	1.00 55.81	A
	ATOM	36	С	ASP A	37	0.356 -25.495	54.728	1.00 41.76	A
	ATOM	37	0	ASP A	37	1.408 -25.659	54.120	1.00 37.74	A
10	ATOM	38	N	LYS A	38	-0.808 -25.976	54.297	1.00 40.27	A
	ATOM	39	CA	LYS A	38	-0.935 -26.728	53.046	1.00 39.95	A
	ATOM	40	СВ	LYS A	38	-2.220 -27.572	53.057	1.00 41.46	A
	MOTA	41	CG	LYS A	38	-2.305 -28.608	54.160	1.00 43.07	A
	ATOM	42	CD	LYS A	38	-1.357 -29.759	53.888	1.00 49.21	A
15	MOTA	43	Œ	LYS A	38	-1.457 -30.840	54.968	1.00 53.99	A
	ATOM	44	NZ	LYS A	38	-0.391 -31.886	54.806	1.00 53.22	A
	ATOM	45	С	LYS A	38	-0.978 -25.770	51.847	1.00 39.66	A
	MOTA	46	0	LYS A	38	-0.533 -26.115	50.757	1.00 39.39	A
	MOTA	47	N	PHE A	39	-1.532 -24.576	52.053	1.00 40.20	A
20	MOTA	48	CA	PHE A	39	-1.628 -23.556	51.001	1.00 37.86	A
	MOTA	49	СВ	PHE A	39	-2.463 -22.362	51.514	1.00 44.93	A
	MOTA	50	CG	PHE A	39	-2.920 -21.388	50.433	1.00 51.45	A
	MOTA	51	CD1	PHE A	39	-2.409 -21.439	49.132	1.00 55.30	A
	MOTA	52	CD2	PHE A	39	-3.866 -20.403	50.731	1.00 51.56	A
25	MOTA	53	CE1	PHE A	39	-2.835 -20.523	48.144	1.00 54.21	Α

	MOTA	54	CE2	PHE A	39	-4.296 -19.485	49.751	1.00 50.99	Α
	MOTA	55	CZ	PHE A	39	-3.779 -19.547	48.460	1.00 51.28	A
	MOTA	56	С	PHE A	39	-0.204 -23.098	50.639	1.00 32.24	Α
	MOTA	57	0	PHE A	39	0.055 -22.637	49.535	1.00 28.40	A
5	MOTA	58	N	LEU A	40	0.719 -23.244	51.580	1.00 29.46	A
	MOTA	59	CA	LEU A	40	2.103 -22.845	51.349	1.00 31.74	Α
	MOTA	60	СВ	LEU A	40	2.952 -23.163	52.579	1.00 32.26	Α
	ATOM _.	61	CG	LEU A	40	2.491 -22.423	53.834	1.00 33.81	Α
	ATOM	62	CD1	LEU A	40	3.404 -22.745	54.998	1.00 35.43	A
10	ATOM	63	CD2	LEU A	40	2.511 -20.906	53.548	1.00 36.44	A
	ATOM	64	С	LEU A	40	2.743 -23.482	50.114	1.00 32.72	Α
	MOTA	65	0	LEU A	40	2.308 -24.546	49.630	1.00 32.75	A
	MOTA	66	N	GLY A	41	3.773 -22.820	49.594	1.00 32.46	A
	MOTA	67	CA	GLY A	41	4.447 -23.356	48.432	1.00 32.86	A
15	ATOM	68	С	GLY A	41	4.363 -22.578	47.134	1.00 33.14	A
	ATOM	69	0	GLY A	41	4.061 -21.380	47.106	1.00 33.14	A
	ATOM	70	N	ARG A	42	4.628 -23.281	46.040	1.00 33.66	A
	MOTA	71	CA	ARG A	42	4.636 -22.665	44.725	1.00 35.33	A
	ATOM	72	СВ	ARG A	42	5.796 -23.233	43.894	1.00 38.39	A
20	ATOM	73	CG	ARG A	42	5.705 -22.932	42.393	1.00 45.57	Α
	ATOM	74	CD	ARG A	42	5.769 -24.211	41.537	1.00 52.54	A
	MOTA	75	NE	ARG A	42	7.141 -24.604	41.210	1.00 57.48	A
	ATOM	76	CZ	ARG A	42	7.486 -25.760	40.643	1.00 60.34	A
	MOTA	77	NH1	ARG A	42	6.564 -26.668	40.334	1.00 61.55	A
25	MOTA	78	NH2	ARG A	42	8.761 -25.998	40.369	1.00 61.04	A

	MOTA	79	С	ARG A	42	3.343 -22.842	43.961	1.00 35.35	A
	MOTA	80	0	ARG A	42	2.838 -23.964	43.821	1.00 35.49	A
	MOTA	81	N :	TRP A	43	2.806 -21.734	43.466	1.00 33.00	A
	MOTA	82	CA	TRP A	43	1.592 -21.791	42.674	1.00 33.72	A
5	MOTA	83	СВ	TRP A	43	0.406 -21.172	43.428	1.00 26.08	A
	MOTA	84	CG	TRP A	43	-0.007 -21.884	44.680	1.00 23.97	A
	MOTA	85	CD2	TRP A	43	-1.096 -22.810	44.818	1.00 22.06	A
	MOTA	86	CE2	TRP A	43	-1.171 -23.169	46.183	1.00 18.60	A
	MOTA	87	CE3	TRP A	43	-2.015 -23.371	43.917	1.00 20.78	A
10	MOTA	88	CD1	TRP A	43	0.529 -21.740	45.936	1.00 25.06	A
	MOTA	89	NE1	TRP A	43	-0.171 -22.508	46.843	1.00 18.01	A
	ATOM	90	CZ2	TRP A	43	-2.128 -24.053	46.669	1.00 23.31	A
	ATOM .	91	CZ3	TRP A	43	-2.964 -24.249	44.400	1.00 24.79	A
	MOTA	92	CH2	TRP A	43	-3.019 -24.583	45.766	1.00 23.79	A
15	ATOM	93	C	TRP A	43	1.826 -21.037	41.358	1.00 35.56	A
	MOTA	94	0	TRP A	43	2.929 -20.550	41.095	1.00 37.26	A
	ATOM	95	N	TYR A	44	0.793 -20.975	40.525	1.00 37.30	A
	ATOM	96	CA	TYR A	44	0.859 -20.248	39.263	1.00 38.32	A
	MOTA	97	CB	TYR A	44	1.120 -21.172	38.072	1.00 39.52	A
20	MOTA	98	CG	TYR A	44	2.402 -21.933	38.138	1.00 40.70	A
	ATOM	99	CD1	TYR A	44	2.402 -23.324	38.354	1.00 38.14	A
	ATOM	100	CE:	1 TYR A	44	3.587 -24.029	38.430	1.00 37.42	A
	ATOM	101	CD:	2 TYR A	44	3.625 -21.274	37.997	1.00 39.25	A
	MOTA	102	CE	2 TYR A	44	4.814 -21.970	38.067	1.00 41.43	A
25	MOTA	103	CZ	TYR A	44	4.792 -23.349	38.286	1.00 41.53	Α

	MOTA	104	OH	TYR A	44	5.985 -24.029	38.370	1.00 45.03	A
	MOTA	105	С	TYR A	44	-0.487 -19.577	39.018	1.00 40.46	Α
	MOTA	106	0	TYR A	44	-1.544 -20.232	39.158	1.00 39.17	A
	MOTA	107	N	SER A	45	-0.433 -18.290	38.657	1.00 40.82	A
5	MOTA	108	CA	SER A	45	-1.618 -17.505	38.318	1.00 43.52	A
	MOTA	109	СВ	SER A	45	-1.243 -16.053	37.994	1.00 44.83	A
	ATOM	110	Œ	SER A	45	-0.342 -15.512	38.936	1.00 52.14	A
	MOTA	111	С	SER A	45	-2.092 -18.152	37.021	1.00 45.66	A
	ATOM	112	0	SER A	45	-1.315 -18.257	36.073	1.00 47.25	A
10	MOTA	113	N	ALA A	46	-3.348 -18.580	36.961	1.00 46.41	A
•	MOTA	114	CA	ALA A	46	-3.850 -19.219	35.748	1.00 45.31	A
	ATOM	115	СВ	ALA A	46	-4.012 -20.698	35.977	1.00 46.81	A
	MOTA	116	С	ALA A	46	-5.166 -18.623	35.296	1.00 45.28	Α
	ATOM	117	0	ALA A	46	-5.489 -18.639	34.113	1.00 48.63	Α
15	MOTA	118	N	GLY A	47	-5.930 -18.104	36.246	1.00 45.61	A
	ATOM	119	CA	GLY A	47	-7.205 -17.511	35.910	1.00 43.75	A
	ATOM	120	С	GLY A	47	-7.329 -16.131	36.505	1.00 43.31	Α
	ATOM	121	0	GLY A	47	-6.677 -15.803	37.485	1.00 44.49	A
	ATOM	122	N	LEU A	48	-8.170 -15.313	35.901	1.00 43.33	A
20	ATOM	123	CA	LEU A	48	-8.396 -13.968	36.384	1.00 43.41	A
	ATOM	124	СВ	LEU A	48	-7.227 -13.074	36.001	1.00 40.63	Α
	MOTA	125	CG	LEU A	48	-6.373 -12.435	37.103	1.00 40.99	A
	MOTA	126	CD1	LEU A	48	-5.112 -11.878	36.455	1.00 38.94	Α
	MOTA	127	CD2	LEU A	48	-7.127 -11.320	37.839	1.00 39.06	Α
25	MOTA	128	С	LEU A	48	-9.675 -13.458	35.741	1.00 46.49	A

	MOTA	129	0	LEU A	48	-9.966 -	-13.752	34.577	1.00 47.60	A
	MOTA	130	N	ALA A	49	-10.442	-12.706	36.515	1.00 49.82	A
	MOTA	131	CA	ALA A	49	-11.687	-12.128	36.043	1.00 54.89	A
	MOTA	132	СВ	ALA A	49	-12.791	-13.149	36.156	1.00 54.30	A
5	MOTA	133	С	ALA A	49	-11.976	-10.916	36.928	1.00 58.99	A
	MOTA	134	О	ALA A	49	-12.011	-11.043	38.155	1.00 61.81	Α
	MOTA	135	N	SER A	50	-12.182	-9.745	36.326	1.00 62.36	A
	MOTA	136	CA	SER A	50	-12.445	-8.550	37.123	1.00 66.74	A
	MOTA	137	СВ	SER A	50	-11.118	-7.939	37.577	1.00 65.83	A
10	MOTA	138	Œ	SER A	50	-11.334	-6.795	38.386	1.00 63.09	A
	MOTA	139	С	SER A	50	-13.284	-7.461	36.456	1.00 70.85	A
	MOTA	140	0	SER A	50	-13.550	-7.511	35.252	1.00 71.11	Α
	MOTA	141	N	ASN A	51	-13.692	-6.480	37.266	1.00 75.09	A
	MOTA	142	CA	ASN A	51	-14.481	-5.331	36.819	1.00 79.23	A
15	MOTA	143	СВ	ASN A	51	-15.582	-4.964	37.824	1.00 81.26	A
	MOTA	144	CG	ASN A	51	-16.260	-6.168	38.435	1.00 84.64	A
	MOTA	145	OD1	ASN A	51	-16.714	-7.072	37.730	1.00 87.24	A
	MOTA	146	ND2	ASN A	51	-16.352	-6.177	39.762	1.00 83.95	A
	MOTA	147	С	ASN A	51	-13.537	-4.137	36.751	1.00 81.34	A
20	MOTA	148	0	ASN A	51	-13.843	-3.120	36.127	1.00 82.27	A
	MOTA	149	N	SER A	52	-12.401	-4.264	37.428	1.00 83.15	A
	MOTA	150	CA	SER A	52	-11.403	-3.205	37.484	1.00 86.71	A
	MOTA	151	СВ	SER A	52	-10.126	-3.725	38.142	1.00 88.84	A
	ATOM	152	Œ	SER A	52	-10.400	-4.259	39.423	1.00 94.06	A
25	MOTA	153	С	SER A	52	-11.052	-2.632	36.125	1.00 88.19	Α

	MOTA	154	0	SER A	52	-10.666	-3.363	35.214	1.00 88.95	A
	MOTA	155	N	SER A	53	-11.191	-1.318	35.989	1.00 90.75	A
	MOTA	156	CA	SER A	53	-10.846	-0.656	34.740	1.00 93.53	A
	MOTA	157	СВ	SER A	53	-10.982	0.863	34.888	1.00 94.58	A
5	MOTA	158	Œ	SER A	53	-10.221	1.345	35.985	1.00 94.06	A
	MOTA	159	С	SER A	53	-9.392	-1.034	34.485	1.00 94.71	A
	MOTA	160	0	SER A	53	-8.986	-1.288	33.350	1.00 94.70	A
	MOTA	161	N	TRP A	54	-8.626	-1.077	35.573	1.00 95.46	A
	MOTA	162	CA	TRP A	54	-7.216	-1.439	35.542	1.00 96.17	A
10	MOTA	163	СВ	TRP A	54	-6.710	-1.638	36.966	1.00 99.29	A
	MOTA	164	CG	TRP A	54	-5.362	-2.259	37.036	1.00103.51	A
	MOTA	165	CD2	TRP A	54	-5.075	-3.654	37.188	1.00107.04	A
	MOTA	166	CE2	TRP A	54	-3.669	-3.795	37.159	1.00108.07	A
	MOTA	167	CE3	TRP A	54	-5.870	-4.801	37.344	1.00107.61	A
15	MOTA	168	CD1	TRP A	54	-4.160	-1.628	36.926	1.00103.66	A
	MOTA	169	NE1	TRP A	54	-3.136	-2.542	36.999	1.00106.47	A
	MOTA	170	CZ2	TRP A	54	-3.035	-5.043	37.281	1.00108.58	A
	MOTA	171	CZ3	TRP A	54	-5.241	-6.043	37.465	1.00107.90	A
	MOTA	172	CH2	TRP A	54	-3.835	-6.151	37.433	1.00107.76	A
20	MOTA	173	С	TRP A	54	-7.044	-2.733	34.759	1.00 95.39	A
	MOTA	174	0	TRP A	54	-6.128	-2.870	33.946	1.00 96.21	A
	ATOM	175	N	PHE A	55	-7.930	-3.684	35.030	1.00 93.38	A
	ATOM	176	CA	PHE A	55	-7.917	-4.975	34.359	1.00 91.11	A
	ATOM	177	СВ	PHE A	55	-8.759	-5.978	35.152	1.00 87.81	A
25	ATOM	178	œ	PHE A	55	-8.933	-7.302	34.469	1.00 82.50	A

	MOTA	179	CD1	PHE A	55	-7.837	-8.109	34.196	1.00 79.44	A
	MOTA	180	CD2	PHE A	55	-10.201	-7.745	34.102	1.00 80.69	A
	MOTA	181	CE1	PHE A	55	-8.001	-9.339	33.569	1.00 78.70	A
	MOTA	182	CE2	PHE A	55	-10.376	-8.971	33.476	1.00 78.47	A
5	MOTA	183	CZ	PHE A	55	-9.275	-9.770	33.208	1.00 78.56	A
	MOTA	184	С	PHE A	55	-8.487	-4.799	32.954	1.00 92.16	A
	MOTA	185	0	PHE A	55	-7.896	-5.255	31.974	1.00 92.45	A
	MOTA	186	N	ARG A	56	-9.638	-4.135	32.867	1.00 92.56	A
	MOTA	187	CA	ARG A	56	-10.285	-3.872	31.586	1.00 92.90	A
10	MOTA	188	СВ	ARG A	56	-11.320	-2.755	31.739	1.00 94.04	A
	MOTA	189	CG	ARG A	56	-12.690	-3.218	32.212	1.00 96.96	A
	MOTA	190	CD	ARG A	56	-13.540	-2.048	32.705	1.00 98.68	A
	MOTA	191	NE	ARG A	56	-14.968	-2.368	32.803	1.00101.63	A
	MOTA	192	CZ	ARG A	56	-15.476	-3.458	33.381	1.00101.88	A
15	MOTA	193	NH1	ARG A	56	-14.682	-4.369	33.927	1.00102.50	A
	MOTA	194	NH2	ARG A	56	-16.790	-3.636	33.421	1.00100.90	A
	MOTA	195	С	ÄRG A	56	-9.227	-3.455	30.572	1.00 92.68	A
	MOTA	196	0	ARG A	56	-9.123	-4.030	29.490	1.00 93.70	A
	MOTA	197	N	GLU A	57	-8.439	-2.452	30.941	1.00 91.14	A
20	MOTA	198	CA	GLU A	57	-7.380	-1.956	30.080	1.00 89.61	A
	MOTA	199	СВ	GLU A	57	-6.835	-0.644	30.631	1.00 90.93	A
	MOTA	200	CG	GLU A	57	-7.913	0.376	30.947	1.00 94.22	A
	MOTA	201	CD	GLU A	57	-7.384	1.576	31.711	1.00 94.94	A
	MOTA	202	OE1	GLU A	57	-8.198	2.461	32.057	1.00 94.57	A
25	MOTA	203	OE2	GLU A	57	-6.160	1.635	31.965	1.00 94.94	A

	MOTA	204	С	GLU A	57	-6.272	-2.991	30.055	1.00 88.82	A
	MOTA	205	0	GLU A	57	-6.254	-3.885	29.207	1.00 89.63	A
	MOTA	206	N	ALA A	58	-5.358	-2.871	31.011	1.00 87.18	A
	MOTA	207	CA	ALA A	58	-4.222	-3.777	31.124	1.00 86.44	A
5	ATOM	208	СВ	ALA A	58	-3.286	-3.285	32.226	1.00 85.99	A
	ATOM	209	С	ALA A	58	-4.621	-5.233	31.389	1.00 84.70	A
	ATOM	210	0	ALA A	58	-4.558	-5.702	32.525	1.00 85.72	A
	MOTA	211	N	LYS A	59	-5.030	-5.946	30.343	1.00 81.60	A
	MOŢA	212	CA	LYS A	59	-5.408	-7.347	30.486	1.00 78.55	A
10	ATOM	213	СВ	LYS A	59	-6.926	-7.496	30.586	1.00 77.93	A
	ATOM	214	CG	LYS A	59	-7.698	-6.993	29.391	1.00 78.22	A
	ATOM	215	CD	LYS A	59	-9.189	-6.930	29.701	1.00 79.39	A
	ATOM	216	Œ	LYS A	59	-9.760	-8.287	30.103	1.00 79.68	A
	ATOM	217	NZ	LYS A	59	-9.769	-9.276	28.990	1.00 78.25	A
15	MOTA	218	С	LYS A	59	-4.880	-8.157	29.317	1.00 78.12	A
	ATOM	219	0	LYS A	59	-5.082	-9.366	29.245	1.00 77.03	A
	ATOM	220	N	ALA A	60	-4.202	-7.479	28.399	1.00 78.69	A
	MOTA	221	CA	ALA A	60	-3.617	-8.137	27.239	1.00 78.11	A
	ATOM	222	СВ	ALA A	60	-3.852	-7.306	25.987	1.00 77.68	A
20	MOTA	223	С	ALA A	60	-2.122	-8.287	27.506	1.00 78.00	A
	ATOM	224	0	ALA A	60	-1.389	-8.895	26.722	1.00 79.90	A
	MOTA	225	N	VAL A	61	-1.683	-7.729	28.629	1.00 76.44	Α
	ATOM	226	CA	VAL A	61	-0.280	-7.787	29.023	1.00 74.53	A
	MOTA	227	СВ	VAL A	61	0.300	-6.361	29.167	1.00 73.76	A
25	MOTA	228	CG1	VAL A	61	0.258	-5.657	27.824	1.00 74.36	A

	MOTA	229	CG2	VAL A	61	-0.497	-5.570	30.199	1.00 71.91	A
	MOTA	230	С	VAL A	61	-0.102	-8.549	30.340	1.00 72.77	A
	MOTA	231	0	VAL A	61	0.669	-8.153	31.214	1.00 72.52	A
	MOTA	232	N	LEU A	62	-0.829	-9.649	30.476	1.00 69.41	A
5	MOTA	233	CA	LEU A	62	-0.752	-10.454	31.680	1.00 64.91	Α
	MOTA	234	СВ	LEU A	62	-2.019	-10.270	32.524	1.00 64.77	Α
	MOTA	235	CG	LEU A	62	-2.228	-8.917	33.220	1.00 64.55	A
	MOTA	236	CD1	LEU A	62	-1.076	-8.658	34.180	1.00 65.57	Α
	MOTA	237	CD2	LEU A	62	-2.319	-7.792	32.191	1.00 65.13	A
10	MOTA	238	С	LEU A	62	-0.555	-11.925	31.354	1.00 61.50	A
	MOTA	239	0	LEU A	62	-1.413	-12.566	30.760	1.00 61.77	A
	MOTA	240	N	TYR A	63	0.600	-12.446	31.738	1.00 57.28	A
	MOTA	241	CA	TYR A	63	0.922	-13.845	31.515	1.00 52.71	Α
	MOTA	242	СВ	TYR A	63	2.378	-14.011	31.031	1.00 57.16	A
15	MOTA	243	CG	TYR A	63	2.705	-13.431	29.663	1.00 61.57	A
	MOTA	244	CD1	TYR A	63	2.613	-12.054	29.423	1.00 60.81	A
• .	MOTA	245	CE1	TYR A	63	2.936	-11.517	28.178	1.00 62.65	A
	MOTA	246	CD2	TYR A	63	3.130	-14.262	28.612	1,00 61.57	A
	MOTA	247	CE2	TYR A	63	3.456	-13.734	27.361	1.00 62.16	A
20	MOTA	248	CZ	TYR A	63	3.357	-12.358	27.152	1.00 64.02	A
	MOTA	249	OH	TYR A	63	3.688	-11.812	25.927	1.00 66.92	A
	MOTA	250	С	TYR A	63	0.782	-14.579	32.845	1.00 48.05	A
	MOTA	251	0	TYR A	63	0.553	-13.970	33.895	1.00 46.41	A
	MOTA	252	N	MET A	64	0.938	-15.895	32.780	1.00 43.07	A
25	MOTA	253	CA	MET A	64	0.885	-16.751	33.949	1.00 37.59	A

	MOTA	254	СВ	MET A	64	1.044 -18.218	33.515	1.00 33.62	A
	MOTA	255	œ	MET A	64	1.270 -19.229	34.631	1.00 34.88	A
	MOTA	256	SD	MET A	64	1.253 -20.956	34.013	1.00 32.69	A
	MOTA	257	CE	MET A	64	-0.441 -21.029	33.468	1.00 29.03	A
5	MOTA	258	С	MET A	64	2.062 -16.304	34.802	1.00 37.67	A
	MOTA	259	0	MET A	64	3.102 -15.923	34.273	1.00 35.70	A
	MOTA	260	N	ALA A	65	1.887 -16.316	36.119	1.00 38.51	A
	MOTA	261	CA	ALA A	65	2.959 -15.928	37.023	1.00 36.56	A
	· MOTA	262	СВ	ALA A	65	2.628 -14.620	37.717	1.00 32.37	A
10	MOTA	263	С	ALA A	65	3.163 -17.012	38.052	1.00 38.63	A
	MOTA	264	0	ALA A	65	2.299 -17.862	38.267	1.00 39.28	A
	MOTA	265	N	LYS A	66	4.332 -16.997	38.672	1.00 41.29	A
	ATOM	266	ĊA	LYS A	66	4.644 -17.962	39.709	1.00 41.75	A
	MOTA	267	СВ	LYS A	66	6.048 -18.539	39.543	1.00 42.34	A
15	MOTA	268	CG	LYS A	66	6.470 -19.366	40.750	1.00 45.37	Α
	MOTA	269	CD	LYS A	66	7.980 -19.398	40.965	1.00 47.49	\mathbf{A}_{\cdot}
	MOTA	270	Œ	LYS A	66	8.674 -20.357	40.013	1.00 50.27	A
	MOTA	271	NZ	LYS A	66	10.093 -20.595.	40.427	1.00 49.08	A
	MOTA	272	С	LYS A	66	4.594 -17.174	40.992	1.00 43.12	A
20	MOTA	273	0	LYS A	66	5.139 -16.072	41.074	1.00 42.51	A
	MOTA	274	N	THR A	67	3.916 -17.723	41.987	1.00 44.36	A
	MOTA	275	CA	THR A	67	3.828 -17.060	43.275	1.00 45.19	A
	MOTA	276	СВ	THR A	67	2.391 -16.536	43.554	1.00 46.71	A
	MOTA	277	OG1	THR A	67	2.030 -15.565	42.566	1.00 48.01	A
25	MOTA	278	CG2	THR A	67	2.308 -15.892	44.930	1.00 46.33	Α

	MOTA	279	С	THR A	67	4.205 -18.087	44.336	1.00 43.89	A
	MOTA	280	0	THR A	67	3.664 -19.195	44.358	1.00 44.64	A
	MOTA	281	N	VAL A	68	5.156 -17.745	45.194	1.00 40.84	A
	MOTA	282	CA	VAL A	68	5.525 -18.679	46.237	1.00 39.30	A
5	MOTA	283	СВ	VAL A	68	7.063 -18.803	46.403	1.00 40.93	A
	MOTA	284	CG1	VAL A	68	7.383 -19.742	47.585	1.00 40.53	A
	MOTA	285	CG2	VAL A	68	7.673 -19.350	45.119	1.00 36.88	A
	MOTA	286	С	VAL A	68	4.882 -18.161	47.505	1.00 36.98	A
	MOTA	287	0	VAL A	68	4.999 -16.981	47.839	1.00 32.83	A
10	MOTA	288	N	VAL A	69 .	4.192 -19.060	48.192	1.00 38.01	A
	MOTA	289	CA	VAL A	69	3.475 -18.722	49.401	1.00 40.63	A
	MOTA	290	СВ	VAL A	69	2.051 -19.349	49.374	1.00 42.62	A
	MOTA	291	CG1	VAL A	69	1.302 -19.042	50.668	1.00 37.81	A
	MOTA	292	CG2	VAL A	69	1.274 -18.813	48.160	1.00 40.66	A
15	MOTA	293	С	VAL A	69	4.191 -19.161	50.662	1.00 41.24	A
	MOTA	294	0	VAL A	69	4.516 -20.337	50.839	1.00 42.46	A
-	MOTA	295	N	ALA A	70	4.423 -18.197	51.542	1.00 40.47	A
	MOTA	296	CA	ALA A	70	5.079 -18.463	52.808	1.00 39.50	A
	MOTA	297	СВ	ALA A	70	6.533 -18.046	52.737	1.00 41.04	A
20	MOTA	298	С	ALA A	70	4.347 -17.669	53.880	1.00 39.27	A
	MOTA	299	0	ALA A	70	3.555 -16.784	53.571	1.00 37.53	A
	MOTA	300	N	PRO A	71	4.578 -18.001	55.156	1.00 39.87	A
	MOTA	301	CD	PRO A	71	5.257 -19.227	55.609	1.00 40.51	A
	MOTA	302	CA	PRO A	71	3.945 -17.321	56.287	1.00 39.82	A
25	MOTA	303	СВ	PRO A	71	4.468 -18.109	57.482	1.00 40.61	A

	MOTA	304	CG	PRO A	71	4.598	-19.485	56.936	1.00 38.21	A
	MOTA	305	С	PRO A	71	4.322	-15.847	56.371	1.00 39.47	A
	MOTA	306	0	PRO A	71	5.402	-15.457	55.928	1.00 41.31	A
	MOTA	307	N	SER A	72	3.437	-15.034	56.940	1.00 39.29	A
5	MOTA	308	CA	SER A	72	3.703	-13.605	57.099	1.00 39.85	A
	MOTA	309	СВ	SER A	72	2.528	-12.765	56.610	1.00 38.06	A
	MOTA	310	œ	SER A	72	1.574	-12.600	57.645	1.00 36.83	A
	MOTA	311	С	SER A	72	3.915	-13.311	58.575	1.00 42.28	A
	MOTA	312	0	SER A	72	3.416	-14.032	59.445	1.00 43.21	A
10	ATOM	313	N	THR A	73	4.629	-12.228	58.851	1.00 44.86	A
	MOTA	314	CA	THR A	73	4.928	-11.823	60.219	1.00 44.43	Α
	ATOM	315	CB	THR A	73	5.477	-10.373	60.271	1.00 42.84	A
	MOTA	316	Œ1	THR A	73	6.640	-10.257	59.439	1.00 41.61	A
	MOTA	317	CG2	THR A	73	5.863	-10.014	61.687	1.00 42.56	A
15	MOTA	318	С	THR A	73	3.748	-11.903	61.179	1.00 45.50	Α
	MOTA	319	0	THR A	73	3.906	-12.321	62.330	1.00 44.76	A
	MOTA	320	N .	GLU A	74	2.568	-11.514	60.707	1.00 47.50	A
	MOTA	321	CA	GLU A	74	1.379	-11.506	61.553	1.00 48.36	A
	MOTA	322	СВ	GLU A	74	0.489	-10.330	61.177	1.00 50.79	A
20	ATOM	323	CG	GLU A	74	-0.323	-9.789	62.322	1.00 59.06	A
	MOTA	324	CD	GLU A	74	0.517	-8.961	63.274	1.00 62.89	A
	MOTA	325	OE1	GLU A	74	0.946	-7.860	62.867	1.00 63.68	A
	MOTA	326	OE2	GLU A	74	0.754	-9.411	64.418	1.00 65.54	A
	MOTA	327	С	GLU A	74	0.547	-12.775	61.510	1.00 47.32	Α
25	MOTA	328	0	GLU A	74	-0.590	-12.786	61.971	1.00 45.23	A

	MOTA	329	N	GLY A	75	1.104 -	13.849	60.967	1.00 48.50	Α
	MOTA	330	CA	GLY A	75	0.338 -	15.076	60.892	1.00 51.57	A
	MOTA	331	С	GLY A	75	-0.492 -	15.094	59.621	1.00 52.32	A
	ATOM	332	O	GLY A	75	-1.429 -	15.884	59.487	1.00 55.22	A
5	MOTA	333	N	GLY A	76	-0.153 -	14.202	58.695	1.00 48.02	A
	MOTA	334	CA	GLY A	76	-0.851 -	14.148	57.429	1.00 41.91	A
	ATOM	335	С	GLY A	76	-0.010 -	14.877	56.400	1.00 39.57	A
	ATOM	336	0	GLY A	76	0.739 -	15.794	56.737	1.00 37.39	A
	ATOM	337	N	LEU A	77	-0.117 -	14.464	55.144	1.00 37.70	A
10	ATOM	338	CA	LEU A	77	0.647 -	15.099	54.085	1.00 35.31	A
	MOTA	339	СВ	LEU A	77	-0.269 -	15.889	53.161	1.00 34.86	A
	ATOM	340	CG	LEU A	77	-1.165 -	16.945	53.809	1.00 37.16	A
	MOTA	341	CD1	LEU A	77	-1.925 -	17.682	52.736	1.00 36.06	A
	ATOM	342	CD2	LEU A	77	-0.326 -	17.909	54.607	1.00 41.20	A
15	MOTA	343	С	LEU A	77	1.425 -	14.120	53.245	1.00 34.86	A
	ATOM	344	0	LEU A	77	0.892 -	13.093	52.831	1.00 36.48	A
	ATOM	345	N	asn a	78	2.697 -	14.450	53.013	1.00 35.83	A
	MOTA	346	CA	asn a	78	3.594 -	13.661	52.173	1.00 34.70	A
	ATOM	347	СВ	asn a	78	5.051 -	13.833	52.588	1.00 35.21	A
20	MOTA	348	CG	ASN A	78	5.513 -	12.770	53.556	1.00 35.91	A
	MOTA	349	OD1	ASN A	78	4.744 -	11.876	53.925	1.00 37.78	A
	ATOM	350	ND2	ASN A	78	6.781 -	12.855	53.972	1.00 34.50	A
	ATOM	351	C.	ASN A	78	3.447 -	14.244	50.799	1.00 36.13	A
	MOTA	352	0	ASN A	78	3.528 -	15.464	50.636	1.00 40.71	A
25	MOTA	353	N	LEU A	79	3.206 -	-13.398	49.810	1.00 36.53	Α

	MOTA	354	CA	LEU A	79	3.088	-13.890	48.448	1.00 40.14	Α
	MOTA	355	СВ	LEU A	79	1.702	-13.583	47.864	1.00 42.52	A
	MOTA	356	CG	LEU A	79	0.678	-14.712	48.099	1.00 43.47	A
	MOTA	357	CD1	LEU A	79 ·	0.435	-14.889	49.586	1.00 42.65	A
5	MOTA	358	CD2	LEU A	79	-0.635	-14.403	47.401	1.00 42.52	A
	MOTA	359	С	LEU A	79	4.185	-13.240	47.638	1.00 40.10	A
	MOTA	360	0	LEU A	79	4.192	-12.023	47.450	1.00 42.17	A
	ATOM	361	N	THR A	80	5.138	-14.058	47.201	1.00 40.26	A
	ATOM	362	CA	THR A	80	6.270	-13.587	46.409	1.00 40.18	A
10	ATOM	363	СВ	THR A	80	7.612	-14.139	46.971	1.00 39.78	A
	MOTA	364	OG1	THR A	80	7.816	-13.649	48.301	1.00 39.20	A
	MOTA	365	CG2	THR A	80	8.779	-13.713	46.104	1.00 38.24	A
	ATOM	366	С	THR A	80	6.069	-14.086	44.990	1.00 40.51	A
	ATOM	367	0	THR A	80	6.047	-15.290	44.745	1.00 39.73	A
15	ATOM	368	N	SER A	81	5.915	-13.165	44.053	1.00 42.62	A
	ATOM	369	CA	SER A	81	5.692	∸13. 569	42.668	1.00 47.88	A
	ATOM	370	СВ	SER A	81	4.310	-13.107	42.205	1.00 47.74	A
	MOTA	371	œ	SER A	81	3.340	-13.307	43.224	1.00 50.44	A
	ATOM	372	С	SER A	81	6.743	-13.071	41.679	1.00 49.35	A
20	MOTA	373	0	SER A	81	7.263	-11.957	41.794	1.00 49.68	A
	MOTA	374	N	THR A	82	7.045	-13.929	40.713	1.00 53.53	A
	MOTA	375	CA	THR A	82	8.001	-13.646	39.655	1.00 57.80	A
	ATOM	376	СВ	THR A	82	9.063	-14.761	39.564	1.00 59.61	A
	ATOM	377	Œ1	THR A	82	9.951	-14.666	40.685	1.00 61.12	A
25	MOTA	378	CG2	THR A	82	9.854	-14.653	38.268	1.00 59.28	A

	MOTA	379	С	THR A	82	7.192	-13.603	38.357	1.00 59.75	A
	MOTA	380	0	THR A	82	6.699	-14.632	37.884	1.00 58.51	A
	MOTA	381	N	PHE A	83	7.050	-12.407	37.793	1.00 62.90	A
	MOTA	382	CA	PHE A	83	6.276	-12.235	36.571	1.00 65.89	A
5	MOTA	383	СВ	PHE A	83	4.961	-11.511	36.871	1.00 61.94	A
	MOTA	384	CG	PHE A	83	5.135	-10.148	37.483	1.00 57.31	A
	MOTA	385	CD1	PHE A	83	4.515	-9.037	36.916	1.00 57.80	A
	MOTA	386	CD2	PHE A	83	5.869	-9.979	38.656	1.00 56.46	A
	MOTA	387	CE1	PHE A	83	4.617	-7.774	37.509	1.00 57.20	A
10	MOTA	388	CE2	PHE A	83	5.979	-8.724	39.257	1.00 57.43	A
	MOTA	389	CZ	PHE A	83	5.351	-7.618	38.683	1.00 58.05	A
	MOTA	390	.C	PHE A	83	6.990	-11.496	35.452	1.00 70.72	A
	MOTA	391	0	PHE A	83	8.068	-10.935	35.639	1.00 71.97	A
	ATOM	392	N	LEU A	84	6.346	-11.501	34.288	1.00 75.56	A
15	MOTA	393	CA	LEU A	84	6.854	-10.856	33.085	1.00 77.58	A
	MOTA	394	СВ	LEU A	84	6.588	-11.760	31.879	1.00 76.28	A
	MOTA	395	CG	LEU A	84	7.137	-11.352	30.513	1.00 75.52	A
	MOTA	396	CD1	LEU A	84	8.635	-11.047	30.622	1.00 76.74	Α
	MOTA	397	CD2	LEU A	84	6.870	-12.481	29.515	1.00 73.55	Α
20	MOTA	398	С	LEU A	84	6.156	-9.517	32.893	1.00 79.65	A
	MOTA	399	0	LEU A	84	4.934	-9.463	32.757	1.00 78.63	A
	MOTA	400	N	ARG A	85	6.933	-8.438	32.899	1.00 84.46	A
	MOTA	401	CA	ARG A	85	6.378	-7.100	32.714	1.00 90.39	A
	MOTA	402	СВ	ARG A	85	6.306	-6.343	34.046	1.00 92.46	A
25	MOTA	403	CG	ARG A	85	5.538	-5.030	33.952	1.00 95.39	A

	MOTA	404	CD	ARG A	85	5.562	-4.245	35.251	1.00 99.40	Α
	MOTA	405	NE	ARG A	85	4.834	-2.982	35.124	1.00103.44	A
	MOTA'	406	CZ	ARG A	85	4.795	-2.037	36.061	1.00105.03	A
	MOTA	407	NH1	ARG A	85	5.445	-2.204	37.207	1.00106.01	A
5	MOTA	408	NH2	ARG A	85	4.105	-0.921	35.852	1.00103.52	A
	MOTA	409	С	ARG A	85	7.237	-6.319	31.726	1.00 92.84	A
	MOTA	410	0	ARG A	85	8.449	-6.178	31.912	1.00 93.32	A
	MOTA	411	N	LYS A	86	6.600	-5.806	30.676	1.00 95.15	A
	MOTA	412	CA	LYS A	86	7.311	-5.059	29.653	1.00 96.71	A
10	MOTA	413	СВ	LYS A	86	7.747	-3.693	30.203	1.00 97.65	A
	MOTA	414	CG	LYS A	86	6.654	-2.621	30.061	1.00 99.15	A
	MOTA	415	CD	LYS A	86	6.720	-1.537	31.131	1.00100.81	A
	MOTA	416	Œ	LYS A	86	6.267	-2.073	32.481	1.00101.99	A
	MOTA	417	NZ	LYS A	86	6.208	-1.012	33.526	1.00102.38	A
15	MOTA	418	С	LYS A	86	8.497	-5.898	29.208	1.00 98.14	A
	MOTA	419	0	LYS A	86	9.621	-5.417	29.080	1.00 97.38	A
	MOTA	420	N	ASN A	87	8.206	-7.180	28.998	1.00101.05	A
	MOTA	421	CA	ASN A	87	9.169	-8.177	28.547	1.00103.17	A
	MOTA	422	СВ	ASN A	87	9.542	-7.902	27.089	1.00105.05	A
20	MOTA	423	CG	ASN A	87	8.322	-7.843	26.180	1.00107.39	A _.
	MOTA	424	OD1	ASN A	87	7.484	-6.946	26.299	1.00107.32	Α
	MOTA	425	ND2	ASN A	87	8.213	-8.809	25.273	1.00109.34	A
	MOTA	426	С	ASN A	87	10.425	-8.279	29.402	1.00103.13	Α
	MOTA	427	0	ASN A	87	10.526	-7.532	30.397	1.00104.41	A
25	MOTA	428	OT	ASN A	87	11.289	-9.117	29.065	1.00101.73	Α

	MOTA	429	С	CYS A	89	11.135	-9.613	35.440	1.00 79.14	A
	MOTA	430	0	CYS A	89	12.261	-9.207	35.721	1.00 79.54	A
	MOTA	431	СВ	CYS A	89	11.946	-11.311	33.779	1.00 82.95	A
	MOTA	432	SG	CYS A	89	11.778	-12.786	34.808	1.00 94.11	Α
5	MOTA	433	N	CYS A	89	10.776	-9.300	32.990	1.00 79.52	A
	MOTA	434	CA	CYS A	89	10.857	-10.295	34.094	1.00 80.27	A
	MOTA	435	N	GLU A	90	10.100	-9.516	36.273	1.00 78.18	A
	MOTA	436	CA	GLU A	90	10.185	-8.842	37.571	1.00 74.49	A
	MOTA	437	СВ	GLU A	90	9.472	-7.495	37.455	1.00 75.68	A
10	MOTA	438	. CG	GLU A	90	9.398	-6.692	38.725	1.00 80.75	A
	MOTA	439	CD ·	GLU A	90	8.770	-5.329	38.509	1.00 83.66	A
	MOTA	440	OE1	GLU A	90	8.511	-4.631	39.519	1.00 87.73	A
	MOTA	441	OE2	GLU A	90	8.540	-4.957	37.334	1.00 80.98	A
	MOTA	442	С	GLU A	90	9.615	-9.632	38.758	1.00 70.33	A
15	MOTA	443	0	GLU A	90	8.910	-10.621	38.581	1.00 69.86	A
	MOTA	444	N	THR A	91	9.928	-9.188	39.971	1.00 66.65	A
	MOTA ,	445	CA	THR A	91	9.446	-9.858	41.176	1.00 64.70	A
	MOTA	446	СВ	THR A	91	10.544	-10.758	41.812	1.00 64.79	A
	MOTA .	447	OG1	THR A	91	10.763	-11.908	40.985	1.00 66.28	A
20	MOTA	448	CG2	THR A	91	10.128	-11.221	43.202	1.00 62.60	A
	MOTA	449	С	THR A	91	8.969	-8.893	42.243	1.00 62.74	A
	MOTA	450	0	THR A	91	9.674	-7.953	42.593	1.00 62.35	A
	MOTA	451	N	LYS A	92	7.775	-9.148	42.767	1.00 61.97	A
	MOTA	452	CA	LYS A	92	7.203	-8.314	43.820	1.00 61.35	A
25	MOTA	453	СВ	LYS A	92	6.190	-7.327	43.234	1.00 64.09	A

	MOTA	454	CG	LYS A	92	6.827	-6.002	42.810	1.00 67.74	A
	MOTA	455	CD	LYS _. A	92	7.705	-5.439	43.933	1.00 69.95	A
	MOTA	456	CE	LYS A	92	6.954	-5.374	45.268	1.00 68.61	A
	MOTA	457	NZ	LYS A	92	7.876	-5.187	46.421	1.00 69.01	A
5	MOTA	458	С	LYS A	92	6.562	-9.113	44.950	1.00 59.21	A
	MOTA	459	0	LYS A	92	6.189	-10.274	44.764	1.00 58.49	A
	MOTA	460	N	ILE A	93	6.433	-8.477	46.116	1.00 57.93	A
	MOTA	461	CA	ILE A	93	5.878	-9.133	47.300	1.00 57.73	A
	MOTA	462	СВ	ILE A	93	6.929	-9.223	48.459	1.00 57.31	A
10	MOTA	463	CG2	ILE A	93	6.352	-10.027	49.624	1.00 53.34	Α
	MOTA	464	CG1	ILE A	93	8.209	-9.921	47.989	1.00 60.14	A
	MOTA	465	CD1	ILE A	93	8.995	-9.163	46.915	1.00 61.98	Α
	ATOM ·	466	C.	ILE A	93	4.638	-8.477	47.891	1.00 57.41	A
	ATOM.	467	0	ILE A	93	4.690	-7.348	48.368	1.00 58.52	A
15	MOTA	468	N	MET A	94	3.526	-9.202	47.872	1.00 57.18	A
	MOTA	469	CA	MET A	94	2.275	-8.716	48.446	1.00 56.08	A
•	MOTA	470	СВ	MET A	94	1.094	-9.102	47.552	1.00 57.29	A
	MOTA	471	CG	MET A	94	1.178	-8.660	46.094	1.00 59.72	A
	ATOM	472	SD	MET A	94	-0.043	-9.548	45.028	1.00 66.73	A
20	MOTA	473	Œ	MET A	94	-1.634	-9.093	45.788	1.00 58.01	Α
	MOTA	474	С	MET A	94	2.141	-9.434	49.799	1.00 57.08	A
	MOTA	475	0	MET A	94	2.504	-10.613	49.914	1.00 58.30	A
	MOTA	476	N	VAL A	95	1.644	-8.738	50.821	1.00 53.57	A
	MOTA	477	CA	VAL A	95	1.460	-9.360	52.130	1.00 49.11	A
25	MOTA	478	СВ	VAL A	95	2.092	-8.543	53.298	1.00 49.18	A

	MOTA	479	CG1	VAL A	95	1.530	-9.046	54.624	1.00 46.36	A
	ATOM	480	CG2	VAL A	95	3.620	-8.677	53.310	1.00 46.36	A
	MOTA	481	С	VAL A	95	-0.012	-9.502	52.452	1.00 48.44	A
	MOTA	482	0	VAL A	95	-0.700	-8.509	52.651	1.00 50.11	A
5	MOTA	483	N	LEU A	96	-0.494	-10.737	52.509	1.00 47.81	A
	MOTA	484	CA	LEU A	96	-1.889	-10.985	52.852	1.00 44.86	A
	MOTA	485	СВ	LEU A	96	-2.347	-12.339	52.306	1.00 44.26	Α
	MOTA	486	CG	LEU A	96	-3.377	-12.254	51.178	1.00 44.31	Α
	MOTA	487	CD1	LEU A	96	-3.072	-11.080	50.245	1.00 45.94	A
10	MOTA	488	CD2	LEU A	96	-3.370	-13.565	50.421	1.00 42.82	A
	MOTA	489	С	LEU A	96	-2.031	-10.968	54.365	1.00 43.84	A
	MOTA	490	0	LEU A	96	-1.466	-11.801	55.070	1.00 42.58	A
	MOTA	491	N	GLN A	97	-2.784	-10.006	54.867	1.00 45.66	A
	MOTA	492	CA	GLN A	97	-2.986	-9.908	56.298	1.00 47.39	A
15	MOTA	493	СВ	GLN A	97	-3.217	-8.451	56.680	1.00 49.05	A
	ATOM	494	CG	GLN A	97	-2.753	-8.111	58.069	1.00 51.88	A
	MOTA	495	CD	GLN A	97	-1.240	-8.117	58.188	1.00 52.17	A
	MOTA	496	OE1	GLN A	97	-0.538	-7.474	57.405	1.00 52.83	A
	MOTA	497	NE2	GLN A	97	-0.732	-8.834	59.177	1.00 51.77	A
20	ATOM	498	С	GLN A	97	-4.187	-10.768	56.713	1.00 48.91	A
	ATOM	499	0	GLN A	97	-5.225	-10.791	56.042	1.00 45.86	A
	MOTA	500	N	PRO A	98	-4.051	-11.506	57.818	1.00 50.41	A
	ATOM	501	CD	PRO A	98	-2.897	-11.599	58.733	1.00 53.20	A
	MOTA	502	CA	PRO A	98	-5.166	-12.347	58.267	1.00 52.85	A
25	ATOM	503	СВ	PRO A	98	-4.566	-13.109	59.456	1.00 54.22	A

	MOTA	504	CG	PRO A 98	-3.519 -12.157	59.986	1.00 54.74	A
	MOTA	505	С	PRO A 98	-6.368 -11.469	58.637	1.00 51.82	A
	MOTA	506	0	PRO A 98	-6.194 -10.401	59.221	1.00 52.75	A
	MOTA	507	N	ALA A 99	-7.578 -11.909	58.291	1.00 50.67	A
5	MOTA	508	CA	ALA A 99	-8.778 -11.123	58.572	1.00 49.91	A
	MOTA	509	СВ	ALA A 99	-9.428 -10.698	57.261	1.00 50.29	A
	MOTA	510	С	ALA A 99	-9.809 -11.808	59.468	1.00 51.08	A
	MOTA	511	0	ALA A 99	-10.991 -11.910	59.125	1.00 51.56	A
	MOTA	512	N	GLY A 100	-9.352 -12.282	60.619	1.00 53.49	A
10	MOTA	513	CA	GLY A 100	-10.245 -12.920	61.569	1.00 55.78	A
	MOTA	514	С	GLY A 100	-10.778 -14.305	61.260	1.00 56.87	A
	MOTA	515	0	GLY A 100	-11.526 -14.869	62.068	1.00 58.84	A
	MOTA	516	N	ALA A 101	-10.418 -14.863	60.111	1.00 55.01	Α
	MOTA	517	CA	ALA A 101	-10.898 -16.197	59.773	1.00 53.78	A
15	MOTA	518	СВ	ALA A 101	-12.313 -16.105	59.194	1.00 51.59	A
	MOTA	519	С	ALA A 101	-9.963 -16.917	58.799	1.00 52.67	A
	MOTA	520	0	ALA A 101	-9.417 -16.302	57.882	1.00 53.80	A
	MOTA	521	N	PRO A 102	-9.760 -18.231	58.997	1.00 50.85	A
	MOTA	522	CD	PRO A 102	-10.339 -19.068	60.065	1.00 49.23	A
20	MOTA	523	CA	PRO A 102	-8.887 -19.024	58.121	1.00 49.90	A
	MOTA	524	СВ	PRO A 102	-9.110 -20.457	58.616	1.00 49.27	A
	MOTA	525	CG	PRO A 102	-9.415 -20.273	60.066	1.00 47.89	A
	MOTA	526	С	PRO A 102	-9.336 -18.841	56.672	1.00 48.42	A
	MOTA	527	0	PRO A 102	-10.544 -18.874	56.405	1.00 49.19	A
25	MOTA	528	N	GLY A 103	-8.383 -18.649	55.752	1.00 45.93	A

	ATOM	529	CA	GLY A	103	-8.726	-18.444	54.342	1.00 45	.39	A
	MOTA	530	С	GLY A	103	-9.323	-17.059	54.045	1.00 45	.32	A
	MOTA	531	0	GLY A	103	-9.872	-16.787	52.963	1.00 42	.49	A
	MOTA	532	N	HIS A	104	-9.202	-16.172	55.025	1.00 43	.72	A
5	MOTA	533	CA	HIS A	104	-9.727	-14.822	54.907	1.00 42	.49	A
	ATOM	534	СВ	HIS A	104	-10.847	7 -14.611	55.926	1.00 43	1.21	Α
	MOTA	535	œ	HIS A	104	-12.10	L -15.334	55.571	1.00 40	0.30	A
	MOTA	536	CD2	HIS A	104	-12.547	7 -16.564	55.914	1.00 42	2.49	A
	ATOM	537	ND1	HIS A	104	-13.028	3 -14.820	54.690	1.00 40).22	A
10	ATOM	538	CE1	HIS A	104	-13.993	3 -15.701	54.504	1.00 43	L.84	A
	MOTA	539	NE2	HIS A	104	-13.724	1 -16.770	55.235	1.00 45	5.92	A
	MOTA	540	С	HIS A	104	-8.621	-13.831	55.142	1.00 41	.81	A
	ATOM	541	Ò	HIS A	104	-8.072	-13.746	56.242	1.00 41	.25	Α
	MOTA	542	N	TYR A	105	-8.285	-13.083	54.107	1.00 41	.35	A
15	ATOM	543	CA	TYR A	105	-7.221	-12.110	54.255	1.00 43	.95	Α
	MOTA	544	CB	TYR A	105	-5.999	-12.584	53.487	1.00 40	.86	A
	MOTA	545	CG	TYR A	105 ·	-5.594	-13.968	53.900	1.00 40	.55	A
	MOTA	546	CD1	TYR A	105	-4.701	-14.167	54.953	1.00 41	.09	A
	MOTA	547	CE1	TYR A	105	-4.358	-15.442	55.362	1.00 41	.55	A
20	ATOM	548	CD2	TYR A	105	-6.138	-15.089	53.265	1.00 38	.66	A
	ATOM	549	CE2	TYR A	105	-5.802	-16.371	53.667	1.00 38	.48	A
	ATOM	550	CZ	TYR A	105	-4.914	-16.545	54.716	1.00 40	.67	A
	MOTA	551	OH	TYR A	105	-4.593	-17.811	55.135	1.00 45	.56	A
	MOTA	552	С	TYR A	105	-7.604	-10.720	53.804	1.00 47	.35	A
25	MOTA	553	0	TYR A	105	-8.684	-10.487	53.249	1.00 48	.78	Α

	MOTA	554	N	THR A 10	6.684	-9.802	54.048	1.00 51.30	A
	MOTA	555	CA	THR A 10	6.857	-8.414	53.683	1.00 52.89	A
	ATOM	556	СВ	THR A 10	06 -7.216	-7.598	54.931	1.00 48.76	A
	MOTA	557	OG1	THR A 10	6 -8.639	-7.407	54.957	1.00 46.67	A
5	MOTA	558	CG2	THR A 10	6.499	-6.270	54.948	1.00 47.39	A
	MOTA	559	С	THR A 10	6 -5.565	-7.937	53.034	1.00 57.01	Α
	MOTA	560	0	THR A 10	06 -4.475	-8.326	53.447	1.00 57.07	Α
	MOTA	561	N	TYR A 10	7 -5.695	-7.106	52.007	1.00 63.36	A
	MOTA	562	CA	TYR A 10	7 -4.530	-6.607	51.293	1.00 72.56	A
10	MOTA	563	CB	TYR A 10	7 -4.409	-7.355	49.968	1.00 73.77	A
	MOTA	564	CG	TYR A 10	7 -3.209	-6.940	49.175	1.00 77.55	A
	ATOM	565	CD1	TYR A 10	7 -1.930	-7.033	49.723	1.00 78.79	A
	MOTA	566	CE1	TYR A 10	-0.816	-6.592	49.023	1.00 81.45	A
	ATOM	567	CD2	TYR A 10	-3.348	-6.400	47.897	1.00 79.21	A
15	ATOM	568	CE2	TYR A 10	7 -2.239	-5.954	47.183	1.00 80.59	A
	MOTA	569	CZ	TYR A 10	0.975	-6.050	47.754	1.00 81.83	A
	MOTA	570	OH	TYR A 10	0.128	-5.593	47.070	1.00 82.92	A
	MOTA	571	С	TYR A 10	7 -4.531	-5.087	51.049	1.00 78.59	A
	MOTA	572	0	TYR A 10	7 -5.565	-4.432	51.172	1.00 80.57	A
20	MOTA	573	N	SER A 10	08 -3.362	-4.541	50.701	1.00 84.94	A
	MOTA	574	CA	SER A 10	08 -3.186	-3.102	50.445	1.00 90.11	A
	MOTA	575	СВ	SER A 10	08 -1.694	-2.750	50.393	1.00 91.85	A
	MOTA	576	Œ	SER A 10	08 -1.053	-3.346	49.277	1.00 92.66	Α
	MOTA	577	C .	SER A 10	08 -3.857	-2.620	49.161	1.00 94.11	A
25	MOTA	578	0	SER A 10	08 -4.755	-3.282	48.644	1.00 95.60	A

	MOTA	579	N	SER A 10	9 -3.413	-1.476	48.637	1.00 98.37	Α
	MOTA	580	CA	SER A 10	9 -4.018	-0.920	47.424	1.00102.82	A
	MOTA	581	СВ	SER A 10	9 -4.804	0.347	47.772	1.00102.05	A
	MOTA	582	œ	SER A 10	9 -3.931	1.407	48.119	1.00101.78	A
5	MOTA	583	С	SER A 10	9 -3.098	-0.603	46.239	1.00106.03	A
	MOTA	584	0	SER A 10	9 -3.205	0.471	45.638	1.00107.26	A
	MOTA	585	N	PRO A 11	0 -2.184	-1.523	45.882	1.00108.55	A
	ATOM	586	CD	PRO A 11	0 -1.863	-2.824	46.492	1.00109.04	A
	MOTA	587	CA	PRO A 11	0 -1.297	-1.253	44.747	1.00109.83	A
10	ATOM	588	СВ	PRO A 11	0 -0.192	-2.281	44.930	1.00109.77	A
	ATOM ·	589	CG	PRO A 11	0 -0.956	-3.452	45.446	1.00109.90	A
	MOTA	590	С	PRO A 11	0 -2.086	-1.467	43.452	1.00110.93	A
	ATOM	591	0	PRO A 11	0 -3.207	-1.985	43.482	1.00110.51	A
	MOTA	592	N	HIS A 11	1 -1.495	-1.087	42.323	1.00111.85	A
15	MOTA	593	CA	HIS A 11	1 -2.161	-1.204	41.028	1.00112.29	A
	MOTA	594	СВ	HIS A 11	1 -2.707	-2.620	40.798	1.00113.17	Α
	MOTA	595	CG	HIS A 11	1 -1.666	-3.696	40.869	1.00115.64	A
	MOTA	596	CD2	HIS A 11	1 -1.106	-4.458	39.901	1.00116.28	Α
	MOTA	597	ND1	HIS A 11	1 -1.092	-4.101	42.055	1.00116.85	Α
20	MOTA	598	CE1	HIS A 11	1 -0.224	-5.067	41.815	1.00117.01	A
	MOTA	599	NE2	HIS A 11	1 -0.213	-5.303	40.514	1.00117.62	A
	MOTA	600	С	HIS A 11	.1 -3.318	-0.214	41.054	1.00112.02	A
	MOTA	601	0	HIS A 11	.1 -3.121	0.994	40.901	1.00111.74	Α
	MOTA	602	N	SER A 11	.2 -4.524	-0.735	41.257	1.00112.13	A
25	MOTA	603	CA	SER A 11	.2 -5.720	0.096	41.332	1.00111.51	A

	MOTA	604	CB	SER A 112	-6.390	0.225	39.958	1.00112.93	Α
	MOTA	605	œ	SER A 112	-7.103	-0.953	39.618	1.00112.49	A
	MOTA	606	С	SER A 112	-6.686	-0.563	42.303	1.00109.76	A
	MOTA	607	0	SER A 112	-7.174	-1.668	42.057	1.00109.39	A
5	ATOM	608	N	GLY A 113	-6.957	0.108	43.414	1.00107.11	A
	MOTA	609	CA	GLY A 113	-7.871	-0.458	44.383	1.00103.45	A
	MOTA	610	С	GLY A 113	-7.781	0.218	45.731	1.00101.21	A
	MOTA	611	0	GLY A 113	-7.451	1.407	45.832	1.00103.49	A
	ATOM	612	N	SER A 114	-8.072	-0.550	46.772	1.00 95.74	A
10	MOTA	613	CA	SER A 114	-8.045	-0.042	48.134	1.00 89.73	A
	MOTA	614	СВ	SER A 114	-9.398	0.595	48.466	1.00 92.13	A
	MOTA	615	œ	SER A 114	-10.475	-0.257	48.097	1.00 94.65	Α
	MOTA	616	С	SER A 114	-7.752	-1.200	49.073	1.00 84.14	Α
	ATOM	617	0	SER A 114	-6.641	-1.714	49.107	1.00 84.52	A
15	MOTA	618	N	ILE A 115	-8.750	-1.605	49.843	1.00 77.31	A
	MOTA	619	CA	ILE A 115	-8.583	-2.725	50.745	1.00 71.63	A
	MOTA	620	СВ	ILE A 115	-9.162	-2.436	52.135	1.00 71.29	Α.
	ATOM	621	CG2	ILE A 115	-8.163	-1.654	52.951	1.00 71.00	A
	MOTA	622	CG1	ILE A 115	-10.488	-1.683	52.001	1.00 73.17	A
20	MOTA	623	CD1	ILE A 115	-11.223	-1.500	53.317	1.00 76.01	A
	ATOM	624	С	ILE A 115	9.311	-3.908	50.139	1.00 68.78	A
	MOTA	625	0	ILE A 115	-10.514	-3.852	49.887	1.00 70.59	À
	MOTA	626	N	HIS A 116	-8.569	-4.973	49.879	1.00 63.17	A
	MOTA	627	CA	HIS A 116	-9.157	-6.162	49.308	1.00 56.48	A
25	ATOM	628	СВ	HIS A 116	-8.219	-6.768	48.269	1.00 52.58	A

	MOTA	629	œ	HIS A 116	-8.046	-5.922	47.048	1.00 52.19	A
	MOTA	630	CD2	HIS A 116	-7.667	-4.630	46.903	1.00 51.18	A
	MOTA	631	ND1	HIS A 116	-8.252	-6.406	45.772	1.00 53.39	A
	ATOM	632	CE1	HIS A 116	-8.006	-5.450	44.894	1.00 52.34	A
5	MOTA	633	NE2	HIS A 116	-7.648	-4.362	45.554	1.00 52.64	A
	MOTA	634	С	HIS A 116	-9.420	-7.166	50.410	1.00 54.37	A
	ATOM	635	0	HIS A 116	-8.579	-7.379	51.273	1.00 56.26	A
	ATOM	636	N	SER A 117	-10.607	-7.754	50.401	1.00 51.47	A
	ATOM	637	CA	SER A 117	-10.952	-8.770	51.381	1.00 48.84	Α
10	ATOM	638	СВ	SER A 117	-12.363	-8.566	51.918	1.00 50.14	A
	ATOM	639	œ	SER A 117	-12.451	-7.332	52.601	1.00 59.59	A
	MOTA	640	С	SER A 117	-10.882	-10.032	50.563	1.00 45.66	Α
	ATOM	641	0	SER A 117	-11.744	-10.289	49.721	1.00 45.39	A
	ATOM	642	N	VAL A 118	-9.832	-10.804	50.800	1.00 42.70	A
15	MOTA	643	CA	VAL A 118	-9.604	-12.030	50.055	1.00 39.83	A
	MOTA	644	СВ	VAL A 118	-8.088	-12.175	49.706	1.00 39.01	A
	ATOM	645	CG1	VAL A 118	-7.839	-13.416	48.830	1.00 34.52	A
	MOTA	646	CG2	VAL A 118	-7.599	-10.907	49.022	1.00 33.42	A
	ATOM	647	С	VAL A 118	-10.068	-13.258	50.826	1.00 38.57	A
20	ATOM	648	0	VAL A 118	-9.781	-13.414	52.030	1.00 35.32	A
	ATOM	649	N	SER A 119	-10.789	-14.124	50.122	1.00 36.68	A
	MOTA	650	CA	SER A 119	-11.289	-15.359	50.718	1.00 36.15	A
	MOTA	651	СВ	SER A 119	-12.798	-15.274	51.001	1.00 33.83	A
	MOTA	652	œ	SER A 119	-13.533	-15.202	49.792	1.00 29.76	A
25	MOTA	653	С	SER A 119	-11.038	-16.501	49.762	1.00 36.50	A

	MOTA	654	0	SER A 1	19	-11.099	-16.336	48.533	1.00	34.43	Α
	MOTA	655	N	VAL A 1	20	-10.760	-17.663	50.340	1.00	36.83	A
	MOTA	656	CA	VAL A 1	20	-10.513	-18.864	49.567	1.00	36.43	A
	MOTA	657	СВ	VAL A 1	20	-9.653	-19.861	50.355	1.00 3	3.61	A
5	MOTA	658	CG1	VAL A 1	20	-9.535	-21.166	49.584	1.00 2	7.88	Α
	MOTA	659	CG2	VAL A 1	20	-8.270	-19.250	50.629	1.00 3	1.31	A
	MOTA	660	С	VAL A 1	20	-11.854	-19.490	49.274	1.00	39.98	A
	MOTA	661	0	VAL A 1	20	-12.484	-20.053	50.170	1.00	42.93	A
	MOTA	662	N	VAL A 1	21	-12.304	-19.385	48.027	1.00	40.55	A
. 10	MOTA	663	CA	VAL A 1	21	-13.593	-19.959	47.654	1.00	41.92	Α
	MOTA	664	СВ	VAL A 1	21	-13.989	-19.551	46.234	1.00	38.14	A
	MOTA	665	CG1	VAL A 1	21	-15.379	-20.125	45.891	1.00	32.71	Α
	MOTA	666	CG2	VAL A 1	21	-13.961	-18.030	46.120	1.00	38.48	Α
•	MOTA	667	С	VAL A 1	21	-13.563	-21.485	47.725	1.00	44.84	A
15	MOTA	668	0	VAL A 1	21	-14.395	-22.103	48.386	1.00	46.44	A
	MOTA	669	N	GLU A 1	22 .	-12.593	-22.080	47.034	1.00	45.48	Α
	MOTA	670	CA	GLU A 1	22	-12.429	-23.527	46.993	1.00	41.76	A
	MOTA	671	СВ	GLU A 1	22	-13.139	-24.092	45.766	1.00	39.34	A
	MOTA	672	CG	GLU A 1	22	-13.627	-25.518	4 5.910	1.00	37.67	A
20	MOTA	673	CD	GLU A 1	22	-14.569	-25.899	44.789	1.00	39.19	Α
	MOTA	674	OE1	GLU A 1	22	-14.093	-26.096	43.656	1.00	43.74	À
	MOTA	675	OE2	GLU A 1	22	-15.789	-25.984	45.028	1.00	39.37	A
	MOTA	676	С	GLU A 1	22	-10.937	-23.749	46.863	1.00	41.01	A
	ATOM	677	0	GLU A 1	22	-10.235	-22.884	46.325	1.00	40.90	A
25	MOTA	678	N	ALA A 1	23	-10.452	-24.890	47.357	1.00	39.08	A

	ATOM	679	CA	ALA A 123	-9.028 -25.191	47.289	1.00 38.09	A
	MOTA	680	СВ	ALA A 123	-8.300 -24.367	48.308	1.00 33.08	A
•	ATOM	681	С	ALA A 123	-8.635 -26.668	47.456	1.00 39.43	A
	ATOM	682	0	ALA A 123	-9.014 -27.323	48.420	1.00 39.20	A
5	MOTA	683	N	ASN A 124	-7.864 -27.170	46.495	1.00 42.59	A
	MOTA	684	CA	ASN A 124	-7.347 -28.532	46.525	1.00 47.72	A
	ATOM	685	СВ	ASN A 124	-7.603 -29.251	45.201	1.00 50.83	A
	ATOM	686	CG	ASN A 124	-7.084 -30.673	45.210	1.00 52.71	A
	ATOM	687	OD1	ASN A 124	-6.047 -30.957	45.809	1.00 54.16	A
10	MOTA	688	ND2	ASN A 124	-7.794 -31.573	44.536	1.00 54.16	A
	MOTA	689	С	ASN A 124	-5.857 -28.278	46.683	1.00 51.11	A
	ATOM	690	0	ASN A 124	-5.143 -28.071	45.699	1.00 51.57	A
	MOTA	691	N	TYR A 125	-5.396 -28.297	47.928	1.00 54.48	A
	ATOM	692	CA	TYR A 125	-4.007 -27.993	48.235	1.00 54.44	A
15	ATOM	693	СВ	TYR A 125	-3.734 -28.230	49.727	1.00 56.30	A
	MOTA	694	CG	TYR A 125	-3.279 -29.620	50.088	1.00 63.82	A
	ATOM	695	CD1	TYR A 125	-4.195 -30.627	50.397	1.00 65.44	A
	ATOM	696	CE1	TYR A 125	-3.760 -31.906	50.761	1.00 68.05	A
	ATOM	697	CD2	TYR A 125	-1.917 -29.925	50.147	1.00 67.54	A
20	ATOM	698	CE2	TYR A 125	-1.472 -31.193	50.504	1.00 69.05	A
	MOTA	699	CZ	TYR A 125	-2.393 -32.179	50.810	1.00 69.43	A
	ATOM	700	OH	TYR A 125	-1.929 -33.430	51.161	1.00 70.34	A
	MOTA	701	С	TYR A 125	-2.930 -28.650	47.365	1.00 53.21	A
	MOTA	702	0	TYR A 125	-1.757 -28.278	47.444	1.00 53.08	A
25	ATOM	703	N	ASP A 126	-3.306 -29.603	46.521	1.00 51.21	A

	MOTA	704	CA	ASP A 12	6 -2.309 -30.229	45.654	1.00 50.82	A
	MOTA	705	СВ	ASP A 12	6 -2.291 -31.746	45.821	1.00 50.35	A
	MOTA	706	CG	ASP A 12	6 -1.829 -32.174	47.178	1.00 51.64	A
	MOTA	707	OD1	ASP A 12	6 -0.687 -31.842	47.557	1.00 57.64	A
5	MOTA	708	OD2	ASP A 12	6 -2.613 -32.851	47.865	1.00 50.91	A
	MOTA	709	С	ASP A 12	6 -2.616 -29.936	44.204	1.00 49.67	A
	MOTA	710	0	ASP A 12	6 -1.801 -30.214	43.321	1.00 49.83	A
	MOTA	711	N	GLU A 12	7 -3.789 -29.356	43.969	1.00 48.57	A
	MOTA	712	CA	GLU A 12	7 -4.249 -29.088	42.613	1.00 47.68	A
10	MOTA	713	СВ	GLU A 12	7 -5.536 -29.886	42.381	1.00 49.84	A
	MOTA	714	CG	GLU A 12	7 -5.846 -30.274	40.949	1.00 53.65	A
	MOTA	715	CD	GLU A 12	7 -7.135 -31.087	40.846	1.00 57.80	A
	MOTA	716	OE1	GLU A 12	7 -7.293 -32.051	41.626	1.00 59.17	A
	MOTA	717	OE2	GLU A 12	7 -7.989 -30.767	39.987	1.00 60.10	A
15	MOTA	718	С	GLU A 12	7 -4.481 -27.619	42.260	1.00 45.31	A
	MOTA	719	0	GLU A 12	7 -3.827 -27.077	41.362	1.00 44.52	A
	MOTA	720	N	TYR A 12	8 -5.397 -26.970	42.970	1.00 41.80	A
	MOTA	721	CA	TYR A 12	8 -5.734 -25.590	42.657	1.00 37.85	A
	MOTA	722	СВ	TYR A 12	8 -6.814 -25.556	41.583	1.00 37.33	A
20	MOTA	723	CG	TYR A 12	8 -8.148 -26.061	42.113	1.00 37.22	A
	MOTA	724	CD1	TYR A 12	8 -8.439 -27.433	42.131	1.00 37.72	A
	MOTA	725	CE1	TYR A 12	8 -9.613 -27.917	42.709	1.00 36.03	A
	MOTA	726	CD2	TYR A 12	8 -9.080 -25.177	42.687	1.00 36.78	A
	MOTA	727	CE2	TYR A 12	8 -10.260 -25.650	43.271	1.00 36.78	A
25	MOTA	728	CZ	TYR A 12	8 -10.517 -27.027	43.278	1.00 38.06	A

	MOTA	729	OH	TYR A 128	-11.661 -27.516	43.867	1.00 38.71	Α
	MOTA	730	С	TYR A 128	-6.283 -24.823	43.842	1.00 38.21	A
	MOTA	731	0	TYR A 128	-6.538 -25.378	44.917	1.00 38.98	A
	MOTA	732	N	ALA A 129	-6.513 -23.536	43.608	1.00 36.38	A
5	MOTA	733	CA	ALA A 129	-7.074 -22.675	44.620	1.00 36.08	A
	MOTA	734	СВ	ALA A 129	-5.979 -22.118	45.531	1.00 33.11	A
	MOTA	735	С	ALA A 129	-7.800 -21.555	43.923	1.00 38.48	A
	MOTA	736	0	ALA A 129	-7.239 -20.857	43.073	1.00 41.82	A
	MOTA	737	N	LEU A 130	-9.068 -21.402	44.269	1.00 39.88	A
10	MOTA	738	CA	LEU À 130	-9.889 -20.353	43.699	1.00 39.61	A
	MOTA	739	СВ	LEU A 130	-11.242 -20.931	43.276	1.00 40.60	· A
	MOTA	740	CG	LEU A 130	-12.118 -20.126	42.305	1.00 43.04	A
	MOTA	741	CD1	LEU A 130	-13.577 -20.402	42.644	1.00 43.37	A
	MOTA	742	CD2	LEU A 130	-11.828 -18.615	42.409	1.00 42.58	A
15	MOTA	743	С	LEU A 130	-10.080 -19.287	44.788	1.00 40.62	A
	MOTA	744	0	LEU A 130	-10.650 -19.571	45.848	1.00 40.06	Α
	ATOM	745	N	LEU A 131	-9.588 -18.073	44.540	1.00 42.77	Α
	MOTA	746	CA	LEU A 131	-9.729 -16.992	45.518	1.00 42.89	A
	ATOM	747	СВ	LEU A 131	-8.394 -16.328	45.830	1.00 42.47	Α
20	MOTA	748	CG	LEU A 131	-7.096 -17.120	45.887	1.00 46.12	A
	MOTA	749	CD1	LEU A 131	-5.972 -16.158	46.240	1.00 45.03	A
	MOTA	750	CD2	LEU A 131	-7.207 -18.267	46.896	1.00 48.77	A
	MOTA	751	С	LEU A 131	-10.648 -15.911	44.995	1.00 43.71	A
	MOTA	752	0	LEU A 131	-10.784 -15.720	43.777	1.00 43.25	A
25	ATOM	753	N	PHE A 132	-11.274 -15.196	45.922	1.00 44.52	Α

	MOTA	754	CA	PHE A	132	-12.156	-14.096	45.560	1.00 44.69	Α
	MOTA	755	СВ	PHE A 1	132	-13.604	-14.419	45.940	1.00 47.03	Α
	MOTA	756	CG	PHE A 1	132	-14.554	-13.278	45.704	1.00 50.56	Α
	MOTA	757	CD1	PHE A 1	132	-14.952	-12.942	44.413	1.00 50.73	Α
5	MOTA	758	CD2	PHE A 1	132	-15.030	-12.518	46.775	1.00 53.02	Α
	MOTA	759	CE1	PHE A 1	132	-15.808	-11.869	44.181	1.00 50.28	Α
	MOTA	760	CE2	PHE A 1	132	-15.885	-11.443	46.558	1.00 53.82	Α
	MOTA	761	CZ	PHE A 1	132	-16.276	-11.116	45.251	1.00 51.52	Α
	MOTA	762	С	PHE A 1	132	-11.685	-12.823	46.277	1.00 43.70	A
10	MOTA	763	0	PHE A 1	132	-11.307	-12.859	47.460	1.00 42.17	A
	MOTA	764	N.	SER A 1	133	-11.704	-11.709	45.549	1.00 41.97	Α
	MOTA	765	CA	SER A 1	133	-11.283	-10.427	46.089	1.00 43.63	Α
		_ : _								
	MOTA	766	CB	SER A 1	L33	-9.939 -	-10.019	45.500	1.00 45.00	A
	MOTA MOTA	766 767	CB CG	SER A 1		-9.939 - -8.966 -		45.500 45.678	1.00 45.00 1.00 51.07	A A
15					133		-11.025			
15	MOTA	767	œ	SER A 1	133 133	-8.966 -	-11.025	45.678	1.00 51.07	A
15	MOTA MOTA	767 768	œ c	SER A 1	133 133 133	-8.966 - -12.288	-11.025 -9.321 -8.972	45.678 45.791	1.00 51.07 1.00 44.02	A A
15	ATOM ATOM	767 768 769	og c o	SER A 1	133 133 133 134	-8.966 - -12.288 -12.542	-11.025 -9.321 -8.972	45.678 45.791 44.641	1.00 51.07 1.00 44.02 1.00 43.30	A A A
15	ATOM ATOM ATOM ATOM	767 768 769 770	OG C O N	SER A 1 SER A 1 SER A 1 ARG A 1	133 133 133 134 134	-8.966 - -12.288 -12.542 -12.852	-11.025 -9.321 -8.972 -8.756	45.678 45.791 44.641 46.841	1.00 51.07 1.00 44.02 1.00 43.30 1.00 46.89	A A A
20	ATOM ATOM ATOM ATOM ATOM	767 768 769 770 771	CCA	SER A 1 SER A 1 ARG A 1 ARG A 1 ARG A 1	133 133 133 134 134	-8.966 - -12.288 -12.542 -12.852 -13.812	-9.321 -8.972 -8.756 -7.679 -8.079	45.678 45.791 44.641 46.841 46.679 47.299	1.00 51.07 1.00 44.02 1.00 43.30 1.00 46.89 1.00 50.11	A A A A
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	767 768 769 770 771 772	CCA CCB	SER A 1 SER A 1 ARG A 1 ARG A 1 ARG A 1	133 133 134 134 134 134	-8.966 -12.288 -12.542 -12.852 -13.812 -15.161	-11.025 -9.321 -8.972 -8.756 -7.679 -8.079 -8.394	45.678 45.791 44.641 46.841 46.679 47.299	1.00 51.07 1.00 44.02 1.00 43.30 1.00 46.89 1.00 50.11 1.00 48.79	A A A A
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	767 768 769 770 771 772 773	CCACCB	SER A 1 SER A 1 ARG A 1 ARG A 1 ARG A 1 ARG A 1	133 133 133 134 134 134 134	-8.966 -12.288 -12.542 -12.852 -13.812 -15.161 -15.081	-9.321 -8.972 -8.756 -7.679 -8.079 -8.394 -9.035	45.678 45.791 44.641 46.841 46.679 47.299 48.774	1.00 51.07 1.00 44.02 1.00 43.30 1.00 46.89 1.00 50.11 1.00 48.79 1.00 44.61	A A A A A
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	767 768 769 770 771 772 773 774	CCACBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	SER A 1 SER A 1 SER A 1 ARG A 1	133 133 133 134 134 134 134	-8.966 -12.288 -12.542 -12.852 -13.812 -15.161 -15.081 -16.347	-11.025 -9.321 -8.972 -8.756 -7.679 -8.079 -8.394 -9.035 -9.372	45.678 45.791 44.641 46.841 46.679 47.299 48.774 49.281	1.00 51.07 1.00 44.02 1.00 43.30 1.00 46.89 1.00 50.11 1.00 48.79 1.00 44.61 1.00 45.37 1.00 48.80	A A A A A
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	767 768 769 770 771 772 773 774 775	CCA CCB CCD NE CCZ	SER A 1 SER A 1 SER A 1 ARG A 1	133 133 134 134 134 134 134 134	-8.966 -12.288 -12.542 -12.852 -13.812 -15.161 -15.081 -16.347 -16.258	-11.025 -9.321 -8.972 -8.756 -7.679 -8.079 -8.394 -9.035 -9.372 -8.480	45.678 45.791 44.641 46.841 46.679 47.299 48.774 49.281 50.700 51.682	1.00 51.07 1.00 44.02 1.00 43.30 1.00 46.89 1.00 50.11 1.00 48.79 1.00 44.61 1.00 45.37 1.00 48.80 1.00 49.92	A A A A A A

	MOTA	779	С	ARG A 13	4 -13.229	-6.450	47.380	1.00 52.29	A
	MOTA	780	0	ARG A 13	4 -12.667	-6.561	48.478	1.00 51.57	A
	MOTA	781	N	GLY A 13	5 -13.341	-5.293	46.729	1.00 51.95	A
	MOTA	782	CA	GLY A 13	5 -12.825	-4.063	47.305	1.00 53.96	A
5	MOTA	783	С	GLY A 13	5 -13.709	-2.884	46.942	1.00 57.08	A
	MOTA	784	0	GLY A 13	5 –14.756	-3.065	46.324	1.00 56.19	A
	MOTA	785	N	THR A 13	6 -13.296	-1.678	47.325	1.00 60.63	A
	MOTA	786	CA	THR A 13	6 -14.070	-0.487	47.004	1.00 64.41	A
	MOTA	787	СВ	THR A 13	6 -15.524	-0.631	47.508	1.00 64.44	A
10	MOTA	788	OG1	THR A 13	6 -16.384	0.228	46.746	1.00 67.53	A
	. MOTA	789	CG2	THR A 13	6 -15.622	-0.267	48.981	1.00 59.31	A
	MOTA	790	С	THR A 13	6 -13.475	0.793	47.590	1.00 66.65	A
	MOTA	791	0	THR A 13	6 -13.016	0.811	48.734	1.00 66.93	Α
	MOTA	792	N	LYS A 13	7 –13.469	1.864	46.800	1.00 68.98	A
15 ·	MOTA	793	CA	LYS A 13	7 -12.963	3.141	47.297	1.00 71.69	Α
	MOTA	794	СВ	LYS A 13	7 -12.422	4.005	46.154	1.00 70.74	A
	MOTA	795	CG	LYS A 13	7 -10.967	3.727	45.804	1.00 70.35	A
	MOTA	796	CD	LYS A 13	7 -10.796	2.436	45.030	1.00 70.21	Α
	MOTA	797	Œ	LYS A 13	7 -11.240	2.603	43.591	1.00 71.89	Α
20	MOTA	798	NZ	LYS A 13	7 -10.407	3.632	42.890	1.00 73.45	Α
	MOTA	799	С	LYS A 13	37 -14.147	3.833	47.965	1.00 73.03	A
	MOTA	800	0	LYS A 13	37 -13.991	4.803	48.723	1.00 74.00	A
	MOTA	801	N	GLY A 13	38 -15.329	3.298	47.675	1.00 71.01	Α
	MOTA	802	CA	GLY A 13	38 -16.562	3.826	48.217	1.00 68.95	A
25	MOTA	803	С	GLY A 13	88 -17.727	3.326	47.386	1.00 68.09	Α

	MOTA	804	0	GLY A 1	.38 –	17.521	2.676	46.360	1.00	64.95	A
	MOTA	805	N	PRO A 1	.39 –	18.968	3.639	47.788	1.00	69.29	A
	MOTA	806	CD	PRO A 1	39 –	19.280	4.704	48.760	1.00	69.05	A
	MOTA	807	CA	PRO A 1	39 -	20.180	3.213	47.075	1.00	68.53	Α
5	MOTA	808	СВ	PRO A 1	39 –	21.285	3.989	47.787	1.00	68.70	Α
	MOTA	809	CG	PRO A 1	39 -	20.575	5.246	48.222	1.00	69.56	Α
	MOTA	810	С	PRO A 1	39 –	20.127	3.519	45.584	1.00	67.82	Α
	MOTA	811	0	PRO A 1	39 –	19.480	4.477	45.165	1.00	70.47	Α
	MOTA	812	N	GLY A 1	40 -	20.805	2.706	44.783	1.00	67.01	Α
10	MOTA	813	CA	GLY A 1	4 0 –	20.805	2.928	43.347	1.00	69.03	A
	MOTA	814	С	GLY A 1	40 -	19.445	2.699	42.710	1.00	70.29	Α
	ATOM	815	0	GLY A 1	40 -	19.263	2.910	41.506	1.00	67.84	Α
	MOTA	816	N	GLN A 1	41 -	18.487	2.269	43.528	1.00	72.03	A
	MOTA	817	CA	GLN A 1	41 -	17.129	1.996	43.069	1.00	73.21	A
15	MOTA	818	СВ	GLN A 1	41 -	16.141	2.874	43.839	1.00	70.86	A
	MOTA	819	CG	GLN A 1	41 -	16.382	4.352	43.607	1.00	69.25	A
	ATOM	820	CD	GLN A 1	41 -	15.226	5.209	44.056	1.00	69.17	Α
	MOTA	821	OE1	GLN A 1	41 -	14.951	5.327	45.249	1.00	69.67	Α
	MOTA	822	NE2	GLN A 1	41 -	14.531	5.807	43.099	1.00	69.51	Α
20	ATOM	823	C .	GLN A 1	41 -	16.793	0.512	43.252	1.00	74.14	A
	ATOM	824	0	GLN A 1	41 -	15.897	-0.033	42.597	1.00	73.63	A
	ATOM	825	N	ASN A 1	42 -	17.532	-0.125	44.153	1.00	74.41	A
	ATOM	826	CA	ASN A 1	.42 –	17.387	-1.541	44.458	1.00	74.91	A
	MOTA	827	СВ	ASN A 1	.42 -	18.714	-2.043	45.033	1.00	77.40	A
25	MOTA	828	CG	ASN A 1	.42 -	18.766	-3.549	45.163	1.00	81.04	A

	MOTA	829	OD1	ASN A 1	142	-19.839	-4.152	45.072	1.00	82.62	A
	MOTA	830	ND2	ASN A 1	142	-17.609	-4.168	45.393	1.00	81.59	A
• **	MOTA	831	С	ASN A 1	142	-16.991	-2.395	43.239	1.00	74.86	Α
	MOTA	832	0	ASN A 1	142	-17.623	-2.322	42.182	1.00	73.84	Α
5	MOTA	833	N	PHE A 1	143	-15.947	-3.206	43.395	1.00	75.81	Α
	MOTA	834	CA	PHE A 1	143	-15.496	-4.084	42.317	1.00	76.18	Α
	MOTA	835	СВ	PHE A 1	143	-14.329	-3.446	41.568	1.00	76.28	Α
	MOTA	836	CG	PHE A 1	143	-13.055	-3.422	42.345	1.00	75.95	Α
	MOTA	837	CD1	PHE A 1	143	-12.237	-4.546	42.396	1.00	74.80	A
10	MOTA	838	CD2	PHE A 1	143	-12.669	-2.274	43.033	1.00	77.92	A
	MOTA	839	CE1	PHE A 1	143	-11.047	-4.528	43.122	1.00	77.10	A
	MOTA	840	CE2	PHE A 1	143	-11.480	-2.241	43.765	1.00	78.61	Α
	MOTA	841	CZ	PHE A 1	143	-10.667	-3.371	43.808	1.00	79.19	A
	MOTA	842	C.	PHE A 1	143	-15.092	-5.476	42.815	1.00	75.21	A
15	MOTA	843	0	PHE A 1	143	-14.874	-5.695	44.008	1.00	74.84	A
	MOTA	844	N	ARG A 1	144	-14.981	-6.407	41.876	1.00	74.55	Α
	MOTA	845	CA	ARG A 1	144	-14.629	-7.790	42.184	1.00	73.79	Α
	MOTA	846	СВ	ARG A 1	144	-15.827	-8.702	41.880	1.00	76.82	A
	MOTA	847	CG	ARG A 1	144	-17.108	-8.334	42.626	1.00	82.57	Α
20	MOTA	848	CD	ARG A	144	-18.340	-8.494	41.732	1.00	88.12	Α
	MOTA	849	NE	ARG A 1	144	-19.588	-8.230	42.457	1.00	92.89	A
·	MOTA	850	CZ	ARG A 1	144	-20.775	-8.046	41.877	1.00	92.42	A
	MOTA	851	NH1	ARG A	144	-20.888	-8.091	40.554	1.00	89.93	A
	MOTA	852	NH2	ARG A	144	-21.852	-7.822	42.624	1.00	90.40	A
25	MOTA	853	С	ARG A	144	-13.411	-8.289	41.399	1.00	70.45	A

	MOTA	854	0	ARG A 144	-12.908	-7.618	40.493	1.00 71.36	Α
	MOTA	855	N	MET A 145	-12.937	-9.475	41.768	1.00 66.18	A
-	MOTA	856	CA	MET A 145	-11.809	-10.100	41.097	1.00 60.85	A
	MOTA	857	СВ	MET A 145	-10.519	-9.310	41.315	1.00 63.62	A
5	MOTA	858	CG	MET A 145	-9.309	-9.999	40.685	1.00 66.34	A
	MOTA	859	SD	MET A 145	-7.851	-8.958	40.573	1.00 70.82	A
	MOTA	860	CE	MET A 145	-7.924	-8.129	42.194	1.00 67.76	A
	MOTA	861	С	MET A 145	-11.607	-11.529	41.564	1.00 56.57	A
	MOTA	862	0	MET A 145	-11.229	-11.780	42.706	1.00 57.01	A
10	MOTA	863	N	ALA A 146	-11.880	-12.467	40.668	1.00 51.49	A
	MOTA	864	CA	ALA A 146	-11.706	-13.876	40.968	1.00 49.13	A
	MOTA	865	СВ	ALA A 146	-12.766	-14.696	40.260	1.00 42.05	A
	MOTA	866	С	ALA A 146	-10.321	-14.252	40.462	1.00 48.78	A
	MOTA	867	0	ALA A 146	-9.869 -	-13.732	39.439	1.00 51.44	Α
15	ATOM	868	N	THR A 147	-9.637 -	-15.136	41.174	1.00 46.49	A
	MOTA	869	CA	THR A 147	-8.318 -	-15.555	40.738	1.00 44.25	A
	MOTA	870	СВ	THR A 147	-7.225 -	-14.925	41.581	1.00 43.85	A
	MOTA	871	OG1	THR A 147	-7.387 -	-13.507	41.573	1.00 49.82	A
	MOTA	872	CG2	THR A 147	-5.864 -	-15.269	41.020	1.00 42.42	A
20	MOTA	873	С	THR A 147	-8.201 -	-17.061	40.838	1.00 44.03	Α
	MOTA	874	0	THR A 147	-8.708 -	-17.668	41.777	1.00 46.81	A
	MOTA	875	N	LEU A 148	-7.534 -	-17.668	39.865	1.00 43.69	A
	MOTA	876	CA	LEU A 148	-7.374 -	-19.111	39.880	1.00 42.50	A
	MOTA	877	СВ	LEU A 148	-8.032 -	-19.731	38.648	1.00 40.72	A
25	MOTA	878	CG	LEU A 148	-7.738 -	-21.228	38.472	1.00 38.40	A

	MOTA	879	CD1	LEU A 14	8 -8.257	-22.027	39.662	1.00 33	3.14	Α
	MOTA	880	CD2	LEU A 14	8 -8.383	-21.700	37.174	1.00 40	0.34	Α
	MOTA	881	С	LEU A 14	8 -5.917	-19.529	39.932	1.00 43	3.54	Α
	MOTA	882	0	LEU A 14	8 -5.172	-19.348	38.964	1.00 41	1.99	Α
5	MOTA	883	N	TYR A 14	9 -5.505	-20.089	41.063	1.00 43	3.29	Α
	MOTA	884	CA	TYR A 14	9 -4.127	-20.529	41.187	1.00 44	4.40	Α
	MOTA	885	СВ	TYR A 14	9 -3.579	-20.188	42.557	1.00 45	5.21	Α
	MOTA	886	CG	TYR A 14	9 -3.203	-18.731	42.702	1.00 50	0.01	Α
	MOTA	887	CD1	TYR A 14	9 -4.145	-17.778	43.094	1.00 54	4.12	A
10	MOTA	888	CE1	TYR A 14	9 -3.784	-16.432	43.272	1.00 58	3.48	A
	MOTA	889	CD2	TYR A 14	9 -1.890	-18.312	42.482	1.00 51	1.47	A
	MOTA	890	CE2	TYR A 14	9 –1.516	-16.982	42.653	1.00 55	5.89	Α
	MOTA	891	CZ	TYR A 14	9 -2.463	-16.045	43.051	1.00 58	3.78	A
	MOTA	892	OH	TYR A 14	9 -2.078	-14.739	43.238	1.00 60	0.02	Α
15	MOTA	893	С	TYR A 14	9 -4.003	-22.025	40.933	1.00 44	1.94	Α
	MOTA	894	0	TYR A 14	9 -4.868	-22.804	41.342	1.00 44	4.18	Α
	MOTA	895	N	SER A 15	0 -2.928	-22.410	40.240	1.00 44	4.38	Α
	MOTA	896	CA	SER A 15	0 -2.668	-23.808	39.914	1.00 41	1.89	Α
	MOTA	897	СВ	SER A 15	0 -2.740	-24.004	38.393	1.00 40	0.38	A
20	MOTA	898	OG ₁	SER A 15	60 -2.579	-25.371	38.026	1.00 40	0.76	Α
	MOTA	899	С	SER A 15	50 -1.297	-24.271	40.428	1.00 40	0.25	Α
	MOTA	900	0	SER A 15	0 -0.342	-23.479	40.500	1.00 39	9.43	Α
	MOTA	901	N	ARG A 15	51 -1.202	-25.547	40.803	1.00 36	6.60	Α
	MOTA	902	CA	ARG A 15	0.074	-26.082	41.259	1.00 34	4.90	Α
25	MOTA	903	СВ	ARG A 15	51 -0.117	-27.347	42.104	1.00 28	8.21	Α

	MOTA	904	CG	ARG A 151	-0.656 -27.122	43.514	1.00 25.36	A
	MOTA	905	CD	ARG A 151	0.340 -26.356	44.388	1.00 23.83	A
•	MOTA	906	NE	ARG A 151	-0.013 -26.412	45.807	1.00 24.06	A
	MOTA	907	CZ	ARG A 151	0.683 -25.813	46.770	1.00 23.10	A
5	MOTA	908	NH1	ARG A 151	1.761 -25.100	46.465	1.00 21.98	A
	MOTA	909	NH2	ARG A 151	0.328 -25.958	48.046	1.00 24.51	A
	MOTA	910	С	ARG A 151	0.890 -26.416	40.015	1.00 35.99	A
	MOTA	911	0	ARG A 151	2.095 -26.617	40.071	1.00 38.57	A
	MOTA	912	N	THR A 152	0.222 -26.458	38.879	1.00 38.62	A
10	MOTA	913	CA	THR A 152	0.893 -26.782	37.631	1.00 41.72	A
	MOTA	914	СВ	THR A 152	0.314 -28.060	37.036	1.00 41.39	A
	MOTA	915	OG1	THR A 152	-1.108 -27.927	36.952	1.00 41.87	A
	MOTA	916	CG2	THR A 152	0.650 -29.253	37.911	1.00 38.85	A
	MOTA	917	С	THR A 152	0.659 -25.647	36.664	1.00 45.58	A
15	ATOM	918	0	THR A 152	-0.238 -24.831	36.878	1.00 51.32	A
	MOTA	919	N	GLN A 153	1.457 -25.573	35.608	1.00 46.22	A
	MOTA	920	CA	GLN A 153	1.273 -24.502	34.637	1.00 47.59	A
	MOTA	921	СВ	GLN A 153	2.577 -24.241	33.902	1.00 43.91	A
	MOTA	922	CG	GLN A 153	3.668 -23.760	34.825	1.00 45.50	A
20	MOTA	923	CD	GLN A 153	5.026 -23.783	34.173	1.00 43.12	A
	MOTA	924	OE1	GLN A 153	5.196 -23.280	33.071	1.00 44.43	A
	MOTA	925	NE2	GLN A 153	6.007 -24.362	34.854	1.00 46.67	A
	MOTA	926	С	GLN A 153	0.170 -24.889	33.666	1.00 52.48	A
	MOTA	927	0	GLN A 153	-0.458 -24.033	33.047	1.00 54.29	A
25	MOTA	928	N	THR A 154	-0.068 -26.190	33.541	1.00 57.63	A

	MOTA	929	CA	THR A 15	4 -1.118 -26.686	32.667	1.00 61.55	A
	MOTA	930	СВ	THR A 15	4 -0.829 -28.128	32.220	1.00 62.65	A
	MOTA	931	Œ1	THR A 15	4 -1.977 -28.654	31.540	1.00 64.17	A
	MOTA	932	CG2	THR A 15	4 -0.491 -29.003	33.426	1.00 60.73	A
5	MOTA	933	С	THR A 15	4 -2.411 -26.652	33.469	1.00 64.71	A
	MOTA	934	0	THR A 15	4 -2.415 -26.973	34.657	1.00 65.83	A
	MOTA	935	N	LEU A 15	5 -3.509 -26.263	32.831	1.00 67.39	A
	MOTA	936	CA	LEU A 15	5 -4.787 -26.179	33.535	1.00 70.46	A
•	MOTA	937	СВ	LEU A 15	5 -5.283 -24.728	33.518	1.00 68.52	A
10 .	MOTA	938	CG	LEU A 15	5 -6.259 -24.291	34.616	1.00 65.62	A
	MOTA	939	CD1	LEU A 15	5 -5.572 -24.339	35.968	1.00 64.23	A
	MOTA	940	CD2	LEU A 15	5 -6.739 -22.881	34.332	1.00 63.47	A
	MOTA	941	С	LEU A 15	5 -5.866 -27.113	32.970	1.00 72.41	A
	MOTA	942	0	LEU A 15	5 -6.189 -27.069	31.782	1.00 74.08	A
15	MOTA	943	N	LYS A 15	6 -6.423 -27.950	33.843	1.00 72.81	A
	MOTA	944	CA	LYS A 15	6 -7.457 -28.917	33.482	1.00 71.61	A
	MOTA	945	СВ	LYS A 15	6 -7.656 -29.861	34.660	1.00 72.76	A
	MOTA	946	CG	LYS A 15	6 -8.563 -31.037	34.411	1.00 75.31	A
	MOTA	947	CD	LYS A 15	66 -8.518 -31.997	35.609	1.00 77.01	A
20	MOTA	948	CE	LYS A 15	66 -7.131 -32.624	35.781	1.00 77.35	A
	ATOM	949	NZ	LYS A 15	66 -7.020 -33.484	36.993	1.00 77.04	A
	ATOM	950	C	LYS A 15	66 -8.771 -28.219	33.125	1.00 71.35	A
	ATOM	951	0	LYS A 15	66 -9.241 -27.357	33.865	1.00 72.68	A
	MOTA	952	N	ASP A 15	-9.368 -28.597	31.997	1.00 70.30	A
25	ATOM	953	CA	ASP A 15	57 -10.617 -27.983	l 31.539	1.00 68.59	A

	MOTA	954	СВ	ASP A	157	-11.173	-28.711	30.308	1.00 68.09	A
	MOTA	955	CG	ASP A	157	-10.446	-28.338	29.028	1.00 68.81	A
	MOTA	956	OD1	ASP A	157	-11.012	-28.564	27.936	1.00 68.86	A
	MOTA	957	OD2	ASP A	157	-9.307	-27.824	29.109	1.00 68.64	A
5	MOTA	958	С	ASP A	157	-11.723	-27.860	32.577	1.00 68.17	A
	MOTA	959	0	ASP A	157	-12.291	-26.779	32.751	1.00 66.02	Α
	MOTA	960	N	GLU A	158	-12.046	-28.957	33.256	1.00 68.99	A
	MOTA	961	CA	GLU A	158	-13.105	-28.904	34.261	1.00 70.32	A
	MOTA	962	СВ	GLU A	158	-13.251	-30.246	34.976	1.00 72.37	A
10	MOTA	963	CG	GLU A	158	-11.947	-30.899	35.372	1.00 78.69	Α
	MOTA	964	CD	GLU A	158	-12.033	-32.419	35.311	1.00 82.57	Α
	MOTA	965	OE1	GLU A	158	-12.844	-33.011	36.061	1.00 81.84	A
	MOTA	966	OE2	GLU A	158	-11.293	-33.022	34.502	1.00 84.84	Α
	MOTA	967	С	GLU A	158	-12.796	-27.807	35.254	1.00 69.10	A
15	MOTA	968	0	GLU A	158	-13.694	-27.178	35.804	1.00 67.41	A
	· MOTA	969	N	LEU A	159	-11.512	-27.569	35.466	1.00 70.39	A
	MOTA	970	CA	LEU A	159	-11.096	-26.521	36.375	1.00 70.62	A
	MOTA	971	СВ	LEU A	159	-9.608 ·	-26.667	36.705	1.00 72.90	A
	MOTA	972	CG	LEU A	159	-9.266 ·	-27.035	38.152	1.00 71.29	A
20 .	MOTA	973	CD1	LEU A	159	-10.266	-28.043	38.713	1.00 73.85	A
	MOTA	974.	CD2	LEU A	159	-7.858 ·	-27.592	38.186	1.00 72.04	A
	MOTA	975	С	LEU A	159	-11.369	-25.177	35.716	1.00 68.60	A
	MOTA	976	0	LEU A	159	-11.785	-24.224	36.375	1.00 68.52	A
	MOTA	977	N	LYS A	160	-11.140	-25.097	34.411	1.00 66.56	A
25	MOTA	978	CA	LYS A	160	-11.395	-23.849	33.714	1.00 66.04	A

	MOTA	979	CB	LYS A 160	-10.941 -23.931	32.254	1.00 66.84	Α
	MOTA	980	œ	LYS A 160	-9.431 -23.947	32.083	1.00 68.12	A
	MOTA	981	CD	LYS A 160	-9.007 -23.675	30.648	1.00 67.76	Α
	MOTA	982	Œ	LYS A 160	-9.354 -24.828	29.727	1.00 68.38	Α
5	MOTA	983	NZ	LYS A 160	-8.843 -24.581	28.352	1.00 69.27	A
	MOTA	984	С	LYS A 160	-12.882 -23.572	33.775	1.00 65.61	Α
	MOTA	985	0	LYS A 160	-13.309 -22.454	34.072	1.00 64.28	A
	MOTA	986	N	GLU A 161	-13.667 -24.609	33.509	1.00 66.07	A
	MOTA	987	CA.	GLU A 161	-15.119 -24.495	33.524	1.00 67.41	A
10	MOTA	988	СВ	GLU A 161	-15.732 -25.852	33.162	1.00 72.11	A
	MOTA	989	CG	GLU A 161	-17.236 -25.860	32.915	1.00 78.85	A
	ATOM	990	CD	GLU A 161	-18.038 -26.299	34.135	1.00 85.16	A
	ATOM	991	OE1	GLU A 161	-17.583 -27.226	34.850	1.00 86.78	A
	MOTA	992	OE2	GLU A 161	-19.130 -25.729	34.366	1.00 85.92	À
15	MOTA	993	С	GLU A 161	-15.574 -24.036	34.907	1.00 64.62	A
	MOTA	994	0	GLU A 161	-16.447 -23.171	35.041	1.00 62.40	A
	ATOM	995	N	LYS A 162	-14.959 -24.607	35.936	1.00 61.68	A
	MOTA	996	CA	LYS A 162	-15.299 -24.255	37.308	1.00 58.49	A
	MOTA	997	СВ	LYS A 162	-14.516 -25.118	38.301	1.00 57.08	Α
20	MOTA	998	œ	LYS A 162	-14.909 -24.877	39.748	1.00 52.74	Α
	MOTA	999	CD	LYS A 162	-13.720 -25.005	40.695	1.00 52.91	A
	MOTA	1000	Œ	LYS A 162	-13.062 -26.378	3 40.620	1.00 54.40	A
	ATOM	1001	NZ	LYS A 162	-13.972 -27.46	4 41.079	1.00 58.06	A
	MOTA	1002	С	LYS A 162	-15.001 -22.79	0 37.582	2 1.00 56.70	A
25	ATOM	1003	0	LYS A 162	-15.753 -22.13	5 38.292	2 1.00 57.73	A

	MOTA	1004	N	PHE A 16	63 -13.89	8 -22.28	5 37.028	1.00 56.10	A
	MOTA	1005	CA	PHE A 16	63 -13.50	5 -20.88	5 37.218	1.00 54.44	A
	MOTA	1006	СВ	PHE A 16	63 -12.08	8 -20.63	8 36.667	1.00 51.03	A
	MOTA	1007	CG	PHE A 16	63 -11.62	0 -19.204	4 36.781	1.00 44.03	A
5	MOTA	1008	CD1	PHE A 16	53 -11.20	3 -18.504	4 35.660	1.00 43.43	A
	MOTA	1009	CD2	PHE A 16	53 -11.57	5 -18.563	38.011	1.00 41.07	Α
	MOTA	1010	CE1	PHE A 16	53 -10.74	3 -17.17	7 35.765	1.00 40.22	A
	MOTA	1011	CE2	PHE A 16	53 -11.11	5 -17.23	38.117	1.00 38.32	A
	MOTA	1012	CZ	PHE A 16	53 -10.70	2 -16.552	2 36.991	1.00 34.24	A
10	MOTA	1013	С	PHE A 16	53 -14.49	4 -19.998	36.482	1.00 56.29	A
	MOTA	1014	0	PHE A 16	53 -14.91	0 -18.958	36.986	1.00 55.86	A
	MOTA	1015	N	THR A 16	54 -14.86	4 -20.429	35.281	1.00 57.68	A
	MOTA	1016	CA	THR A 16	54 -15.80	7 -19.694	4 34.465	1.00 59.18	A
	MOTA	1017	СВ	THR A 16	54 -16.10	3 -20.449	9 33.167	1.00 62.54	A
15	MOTA	1018	OG1	THR A 16	54 -14.88	7 -20.598	32.418	1.00 66.72	A
	MOTA	1019	CG2	THR A 16	5 4 - 17.1 3	7 -19.693	1 32.325	1.00 64.98	A
	MOTA	1020	С	THR A 16	64 -17.10	2 -19.525	5 35.228	1.00 58.45	A
	MOTA	1021	0	THR A 16	64 -17.55	0 -18:408	35.484	1.00 58.64	A
	MOTA	1022	N	THR A 16	65 -17.69	7 -20.650	35.590	1.00 57.76	A
20	MOTA	1023	CA	THR A 16	65 -18.94	9 -20.653	3 36.326	1.00 57.32	A
	MOTA	1024	СВ	THR A 16	65 -19.30	0 -22.068	36.809	1.00 59.13	A
	MOTA	1025	OG1	THR A 16	65 -19.42	3 -22.945	5 35.681	1.00 60.25	A
	MOTA	1026	CG2	THR A 16	65 –20.60	0 -22.058	37.575	1.00 59.06	A
	MOTA	1027	С	THR A 16	65 -18.88	2 -19.73	5 37.533	1.00 55.51	A
25	MOTA	1028	0	THR A 16	65 -19.75	6 -18.88	4 37.722	1.00 53.88	A

	MOTA	1029	N	PHE A 166	-17.852 -1	9.899 38.	357 1.00	55.03	Α
	MOTA	1030	CA	PHE A 166	-17.748 -1	9.052 39.	529 1.00	56.67	A
	MOTA	1031	СВ	PHE A 166	-16.520 -1	9.373 40.	372 1.00	55.47	A
	MOTA	1032	CG	PHE A 166	-16.287 -1	8.365 41.	467 1.00	55.56	A
5	MOTA	1033	CD1	PHE A 166	-17.173 -1	8.270 42.	548 1.00	55.01	A
	MOTA	1034	CD2	PHE A 166	-15.252 -1	7.435 41.	369 1.00	52.09	A
	MOTA	1035	CE1	PHE A 166	-17.036 -1	7.250 43.	522 1.00	49.17	A
	MOTA	1036	CE2	PHE A 166	-15.108 -1	6.416 42.	331 1.00	50.06	A
	MOTA	1037	CZ	PHE A 166	-16.007 -1	6.326 43.	408 1.00	48.33	A
10	MOTA	1038	С	PHE A 166	-17.664 -1	7.600 39.	112 1.00	58.10	A
	MOTA	1039	0	PHE A 166	-18.306 -1	6.739 39.	709 1.00	58.87	A
	MOTA	1040	N	SER A 167	-16.856 -1	7.347 38.	089 1.00	59.52	Α
	MOTA	1041	CA	SER A 167	-16.647 -1	6.007 37.	561 1.00	61.95	Α
•	MOTA	1042	СВ	SER A 167	-15.751 -1	6.070 36.	320 1.00	64.01	A
15	MOTA	1043	œ	SER A 167	-14.496 -1	6.670 36.	603 1.00	68.65	Α
	MOTA	1044	С	SER A 167	-17.969 -1	5.342 37.	195 1.00	62.37	Α
	MOTA	1045	Ο	SER A 167	-18.236 -1	4.203 37.	576 1.00	60.74	A
	MOTA	1046	N	LYS A 168	-18.794 -1	6.059 36.	445 1.00	64.25	Α
	MOTA	1047	CA	LYS A 168	-20.079 -1	5.519 36.	032 1.00	65.94	A
20	MOTA	1048	СВ	LYS A 168	-20.693 -1	6.374 34.	918 1.00	68.53	Α
	MOTA	1049	CG	LYS A 168	-19.931 -1	6.315 33.	592 1.00	70.35	A
	MOTA	1050	CD	LYS A 168	-20.558 -1	7.226 32.	537 1.00	72.07	A
	MOTA	1051	CE	LYS A 168	-19.737 -1	7.228 31.	250 1.00	74.35	A
	MOTA	1052	NZ	LYS A 168	-20.251 -1	8.206 30.	238 1.00	76.09	A
25	MOTA	1053	С	LYS A 168	-21.016 -1	5.454 37.	222 1.00	65.80	A

	MOTA	1054	0	LYS A 16	58 -21.728	-14.467	37.399	1.00	65.98	Α
	MOTA	1055	N	GLY A 16	59 –21.000	-16.502	38.045	1.00	65.48	A
	MOTA	1056	CA	GLY A 16	59 -21.851	-16.528	39.220	1.00	62.40	A
	MOTA	1057	С	GLY A 16	59 -21.627	-15.302	40.088	1.00	62.09	Α
5	MOTA	1058	0	GLY A 16	59 -22.241	-15.164	41.141	1.00	64.40	A
	MOTA	1059	N	GLN A 17	70 -20.764	-14.394	39.641	1.00	60.28	Α
	MOTA	1060	CA	GLN A 17	70 -20.455	-13.202	40.410	1.00	60.01	Α
	MOTA	1061	СВ	GLN A 17	70 -19.000	-13.268	40.878	1.00	60.09	A
	MOTA	1062	CG	GLN A 17	70 -18.720	-14.443	41.797	1.00	59.29	A
10	MOTA	1063	CD	GLN A 17	70 -19.396	-14.276	43.144	1.00	60.40	A
	MOTA	1064	OE1	GLN A 17	70 -19.838	-15.255	43.766	1.00	58.57	A
	MOTA	1065	NE2	GLN A 17	70 -19.472	-13.028	43.612	1.00	56.49	A
	MOTA	1066	С	GLN A 17	70 –20.688	-11.920	39.631	1.00	61.05	A
	MOTA	1067	0	GLN A 17	70 -20.510	-10.825	40.159	1.00	58.93	A
15	MOTA	1068	N	GLY A 17	71 -21.085	-12.059	38.373	1.00	64.02	A
	MOTA	1069	CA	GLY A 17	71 -21.325	-10.884	37.560	1.00	69.34	A
	MOTA	1070	С	GLY A 17	71 -20.146	-10.546	36.667	1.00	72.57	A
	MOTA	1071	0	GLY A 17	71 -19.940	-9.388	36.293	1.00	73.44	Α
	MOTA	1072	N	LEU A 17	72 –19.356	-11.558	36.332	1.00	74.78	A
20	MOTA	1073	CA	LEU A 17	72 -18.211	-11.369	35.455	1.00	76.66	Α
	MOTA	1074	СВ	LEU A 17	72 -16.941	-11.959	36.082	1.00	76.52	A
	MOTA	1075	CG	LEU A 17	72 -16.304	-11.200	37.255	1.00	75.12	Α
	MOTA	1076	CD1	LEU A 17	72 -15.622	-9.945	36.746	1.00	74.02	A
	MOTA	1077	CD2	LEU A 17	72 -17.363	-10.852	38.295	1.00	76.24	A
25	MOTA	1078	С	LEU A 17	72 -18.551	-12.095	34.166	1.00	77.94	A

	MOTA	1079	0	LEU A	172	-18.950	-13.261	34.192	1.00	78.67	A
	MOTA	1080	N	THR A	173	-18.410	-11.407	33.039	1.00	78.36	A
	MOTA	1081	CA	THR A	173	-18.727	-12.017	31.755	1.00	79.91	A
	MOTA	1082	СВ	THR A	173	-19.248	-10.989	30.752	1.00	80.74	A
5	MOTA	1083	OG1	THR A	173	-18.138	-10.416	30.051	1.00	82.51	Α
	MOTA	1084	CG2	THR A	173	-20.021	-9.888	31.467	1.00	81.84	A
	MOTA	1085	С	THR A	173	-17.516	-12.679	31.130	1.00	79.82	A
	MOTA	1086	0	THR A	173	-16.417	-12.653	31.684	1.00	80.17	A
	MOTA	1087	N	GLU A	174	-17.732	-13.257	29.955	1.00	80.54	A
10	MOTA	1088	CA	GLU A	174	-16.681	-13.945	29.222	1.00	82.10	A
	MOTA	1089	СВ	GLU A	174	-17.261	-14.552	27.940	1.00	85.56	A
	MOTA	1090	CG	GLU A	174	-16.541	-15.799	27.443	1.00	89.66	A
	MOTA	1091	CD	GLU A	174	-16.562	-16.933	28.460	1.00	92.42	A
	MOTA	1092	OE1	GLU A	174	-15.909	-16.798	29.520	1.00	94.51	Α
15	MOTA	1093	OE2	GLU A	174	-17.235	-17.957	28.204	1.00	93.50	Ą
	MOTA	1094	С	GLU A	174	-15.543	-12.991	28.880	1.00	79.44	A
	MOTA	1095	0	GLU A	174	-14.371	-13.358	28.932	1.00	77.18	A
	MOTA	1096	N	GLU A	175	-15.896	-11.760	28.535	1.00	77.88	A
	MOTA	1097	CA	GLU A	175	-14.897	-10.764	28.188	1.00	76.60	A
20	MOTA	1098	СВ	GLU A	175	-15.569	-9.498	27.662	1.00	78.33	A
	ATOM	1099	CG	GLU A	175	-16.347	-8.749	28.723	1.00	82.41	A
	MOTA	1100	CD	GLU A	175	-16.962	-7.465	28.209	1.00	84.48	A
	MOTA	1101	OE1	GLU A	175	-16.204	-6.555	27.819	1.00	86.80	A
	MOTA	1102	OE2	GLU A	175	-18.207	-7.365	28.198	1.00	84.05	A
25	ATOM	1103	С	GLU A	175	-14.047	-10.412	29.399	1.00	74.57	A

	MOTA	1104	0	GLU A 175	-13.009 -9.772	29.259	1.00 75.53	Α
	MOTA	1105	N	ASP A 176	-14.486 -10.818	30.587	1.00 72.84	A
-	MOTA	1106	CA	ASP A 176	-13.737 -10.525	31.808	1.00 71.42	A
	MOTA	1107	СВ	ASP A 176	-14.680 -10.222	32.974	1.00 72.57	A
5	ATOM	1108	œ	ASP A 176	-15.839 -9.341	32.576	1.00 74.87	A
	MOTA	1109	OD1	ASP A 176	-16.734 -9.846	31.873	1.00 74.74	A
	MOTA	1110	OD2	ASP A 176	-15.853 -8.150	32.963	1.00 75.76	A
	MOTA	1111	С	ASP A 176	-12.855 -11.700	32.203	1.00 69.16	A
	MOTA	1112	0	ASP A 176	-11.823 -11.530	32.841	1.00 69.29	A
10	MOTA	1113	N	ILE A 177	-13.275 -12.894	31.817	1.00 67.03	A
	MOTA	1114	CA	ILE A 177	-12.545 -14.101	32.150	1.00 66.00	A
	ATOM	1115	СВ	ILE A 177	-13.477 -15.311	32.114	1.00 66.64	A
	MOTA	1116	CG2	ILE A 177	-12.815 -16.492	32.806	1.00 66.54	A
	MOTA	1117	CG1	ILE A 177	-14.796 -14.959	32.802	1.00 67.72	A
15	MOTA	1118	CD1	ILE A 177	-15.848 -16.051	32.702	1.00 70.45	A
	MOTA	1119	С	ILE A 177	-11.370 -14.364	31.218	1.00 65.75	A
	MOTA	1120	0	ILE A 177	-11.546 -14.700	30.045	1.00 67.30	A
	MOTA	1121	N	VAL A 178	-10.166 -14.224	31.756	1.00 63.32	A
	MOTA	1122	CA	VAL A 178	-8.955 -14.447	30.985	1.00 59.20	A
20	MOTA	1123	CB	VAL A 178	-8.006 -13.243	31.082	1.00 58.03	A
	MOTA	1124	CG1	VAL A 178	-6.856 -13.419	30.114	1.00 60.86	A
	MOTA	1125	CG2	VAL A 178	-8.755 -11.962	30.803	1.00 58.82	A
•	MOTA	1126	С	VAL A 178	-8.201 -15.646	31.529	1.00 56.79	A
	MOTA	1127	0	VAL A 178	-8.326 -15.993	32.698	1.00 59.10	A
25	MOTA	1128	N	PHE A 179	-7.419 -16.284	30.680	1.00 55.88	Α

	MOTA	1129	CA	PHE A 179	-6.607 -17.401	31.127	1.00 56.34	Α
	ATOM	1130	СВ	PHE A 179	-7.052 -18.707	30.483	1.00 53.11	A
	MOTA	1131	CG	PHE A 179	-8.356 -19.202	31.007	1.00 53.55	A
	MOTA	1132	CD1	PHE A 179	-9.548 -18.869	30.373	1.00 52.88	A
5	MOTA	1133	CD2	PHE A 179	-8.401 -19.980	32.162	1.00 55.37	A
	MOTA	1134	CE1	PHE A 179	-10.771 -19.305	30.878	1.00 51.85	A
	ATOM	1135	CE2	PHE A 179	-9.619 -20.423	32.680	1.00 54.21	A
	MOTA	1136	CZ	PHE A 179	-10.809 -20.084	32.034	1.00 54.72	A
	MOTA	1137	С	PHE A 179	-5.175 -17.082	30.771	1.00 56.94	A
10	MOTA	1138	0	PHE A 179	-4.750 -17.224	29.629	1.00 58.94	A
	MOTA	1139	N	LEU A 180	-4.444 -16.616	31.770	1.00 56.14	A
	MOTA	1140	CA	LEU A 180	-3.060 -16.233	31.596	1.00 57.47	A .
	MOTA	1141	СВ	LEU A 180	-2.437 -15.987	32.963	1.00 57.31	A
	MOTA	1142	CG	LEU A 180	-3.361 -15.108	33.810	1.00 56.20	A
15	MOTA	1143	CD1	LEU A 180	-3.093 -15.359	35.294	1.00 55.59	A
	MOTA	1144	CD2	LEU A 180	-3.185 -13.645	33.424	1.00 52.11	A
	MOTA	1145	С	LEU A 180	-2.274 -17.288	30.843	1.00 58.94	A
	MOTA	1146	0	LEU A 180	-2.327 -18.472	31.176	1.00 59.95	A
	ATOM	1147	N	PRO A 181	-1.549 -16.867	29.799	1.00 60.40	A
20	ATOM	1148	CD	PRO A 181	-1.633 -15.518	29.208	1.00 59.15	A
	MOTA	1149	CA	PRO A 181	-0.727 -17.741	28.961	1.00 63.62	A
	MOTA	1150	СВ	PRO A 181	-0.619 -16.953	27.666	1.00 61.46	A
	ATOM	1151	CG	PRO A 181	-0.533 -15.549	28.166	1.00 57.89	A
	ATOM	1152	С	PRO A 181	0.640 -17.966	29.598	1.00 67.50	A
25	ATOM	1153	0	PRO A 181	1.154 -17.086	30.284	1.00 68.06	A

	MOTA	1154	N	GLN A 182	1.223 -19.138	29.364	1.00 70.91	A
	MOTA	1155	CA	GLN A 182	2.538 -19.458	29.912	1.00 74.68	A
. • .	MOTA	1156	СВ	GLN A 182	2.945 -20.894	29.570	1.00 74.56	A
	MOTA	1157	œ	GLN A 182	1.933 -21.971	29.892	1.00 76.21	A
5	MOTA	1158	CD	GLN A 182	2.520 -23.373	29.728	1.00 77.21	A
	MOTA	1159	OE1	GLN A 182	1.790 -24.364	29.679	1.00 77.14	A
	MOTA	1160	NE2	GLN A 182	3.848 -23.458	29.655	1.00 74.73	A
	MOTA	1161	С	GLN A 182	3.599 -18.527	29.329	1.00 77.11	A
	ATOM	1162	0	GLN A 182	3.851 -18.546	28.127	1.00 77.72	Α
10	MOTA	1163	N	PRO A 183	4.232 -17.696	30.169	1.00 79.26	A
	ATOM	1164	CD	PRO A 183	3.959 -17.395	31.585	1.00 78.43	A
	MOTA	1165	CA	PRO A 183	5.260 -16.800	29.637	1.00 82.07	A
	MOTA	1166	СВ	PRO A 183	5.334 -15.706	30.691	1.00 79.37	A
	ATOM	1167	CG	PRO A 183	5.106 -16.472	31.944	1.00 78.09	A
15	MOTA	1168	С	PRO A 183	6.576 -17.567	29.497	1.00 86.60	A
	MOTA	1169	0	PRO A 183	7.309 -17.743	30.474	1.00 88.58	A
	MOTA	1170	N	ASP A 184	6.856 -18.037	28.285	1.00 89.35	A
	MOTA	1171	CA	ASP A 184	8.074 -18.790	27.996	1.00 91.71	A
	MOTA	1172	СВ	ASP A 184	8.376 -18.720	26.496	1.00 90.76	A
20	MOTA	1173	CG	ASP A 184	8.268 -17.308	25.946	1.00 91.18	A
	MOTA	1174	OD1	ASP A 184	9.028 -16.421	26.394	1.00 92.29	A
	MOTA	1175	OD2	ASP A 184	7.415 -17.080	25.064	1.00 91.05	A
	MOTA	1176	С	ASP A 184	9.287 -18.298	28.786	1.00 93.40	A
	ATOM	1177	0	ASP A 184	10.143 -19.090	29.187	1.00 93.35	A
25	MOTA	1178	N	LYS A 185	9.347 -16.989	29.014	1.00 95.42	A

	MOTA	1179	CA	LYS A 185	10.451 -16.376	29.744	1.00 95.83	Α
	MOTA	1180	СВ	LYS A 185	10.661 -14.943	29.239	1.00 96.46	A
	MOTA	1181	CG	LYS A 185	11.974 -14.287	29.659	1.00 98.21	A
	MOTA	1182	CD	LYS A 185	12.077 -12.872	29.092	1.00100.88	A
5	MOTA	1183	CE	LYS A 185	13.448 -12.250	29.335	1.00102.05	A
	MOTA	1184	NZ	LYS A 185	13.760 -12.116	30.785	1.00104.65	A
	MOTA	1185	С	LYS A 185	10.192 -16.366	31.250	1.00 95.82	A
	MOTA	1186	0	LYS A 185	9.619 -17.299	31.804	1.00 94.92	A
	MOTA	1187	N	CYS A 186	10.627 -15.291	31.890	1.00 96.28	A
10	MOTA	1188	CA	CYS A 186	10.492 -15.074	33.321	1.00 97.57	A
	MOTA	1189	С	CYS A 186	10.358 -16.297	34.239	1.00 99.39	A
	MOTA	1190	0	CYS A 186	11.328 -16.685	34.887	1.00100.13	A
	MOTA	1191	СВ	CYS A 186	9.352 -14.098	33.575	1.00 95.95	A
	MOTA	1192	SG	CYS A 186	9.759 -13.012	34.968	1.00 98.27	A
15	MOTA	1193	N	ILE A 187	9.171 -16.889	34.324	1.00101.87	A
	MOTA	1194	CA	ILE A 187	8.976 -18.066	35.175	1.00103.65	A
	MOTA	1195	СВ	ILE A 187	7.513 -18.517	35.189	1.00100.55	A
	MOTA	1196	CG2	ILE A 187	7.375 -19.795	35.996	1.00100.83	A
	MOTA	1197	CG1	ILE A 187	6.631 -17.417	35,765	1.00 97.38	A
20	MOTA	1198	CD1	ILE A 187	5.172 -17.755	35.710	1.00 94.71	A
	MOTA	1199	С	ILE A 187	9.805 -19.235	34.659	1.00107.87	A
	MOTA	1200	0	ILE A 187	10.074 -19.324	33.463	1.00109.90	A
	MOTA	1201	N	GLN A 188	10.193 -20.138	35.554	1.00111.72	A
	MOTA	1202	CA	GLN A 188	10.998 -21.296	35.168	1.00116.09	A
25	ATOM	1203	СВ	GLN A 188	11.467 -22.053	36.412	1.00117.84	Α

	MOTA	1204	CG	GLN A	188	12.347	-21.230	37.335	1.00120.37	A
	MOTA	1205	CD	GLN A	188	13.626	-20.764	36.665	1.00120.88	A
	MOTA	1206	OE1	GLN A	188	13.592	-20.088	35.637	1.00121.37	A
	MOTA	1207	NE2	GLN A	188	14.763	-21.121	37.250	1.00120.87	A
5	MOTA	1208	С	GLN A	188	10.251	-22.249	34.241	1.00118.05	A
	MOTA	1209	0	GLN A	188	9.512	-23.125	34.696	1.00118.11	A
	MOTA	1210	N	GLU A	189	10.462	-22.070	32.938	1.00120.59	A
	MOTA	1211	CA	GLU A	189	9.830	-22.892	31.904	1.00121.84	A
	MOTA	1212	СВ	GLU A	189	10.296	-24.352	32.015	1.00122.00	Α
10	MOTA	1213	CG	GLU A	189	10.004	-25.210	30.781	1.00120.78	A
	MOTA	1214	CD	GLU A	189	10.895	-24.865	29.600	1.00120.07	A
	MOTA	1215	OE1	GLU A	189	10.855	-23.705	29.142	1.00119.99	A
	MOTA	1216	OE2	GLU A	189	11.636	-25.753	29.129	1.00120.26	Α
	MOTA	1217	С	GLU A	189	8.308	-22.830	32.001	1.00122.03	A
15	MOTA	1218	0	GLU A	189	7.697	-23.870	32.332	1.00121.94	A
	MOTA	1219	OT	GLU A	189	7.748	-21.740	31.749	1.00121.99	A
	MOTA	1220	OH2	WAT W	200	6.622	-15.627	50.105	1.00 32.46	W
	MOTA	1221	OH2	WAT W	201	-13.735	5 -12.460	49.782	1.00 32.29	W
	MOTA	1222	OH2	WAT W	203	-15.181	-17.532	49.376	1.00 37.27	W
20	MOTA	1223	OH2	WAT W	204	-15.122	2 -18.405	51.994	1.00 34.03	W
	MOTA	1224	OH2	WAT W	205	-11.282	2 -24.928	56.736	1.00 73.37	W
	MOTA	1225	OH2	WAT W	206	1.440	-10.333	58.570	1.00 44.34	W
	MOTA	1226	OH2	WAT W	207	-6.812	-15.884	58.098	1.00 42.35	W
	MOTA	1227	OH2	WAT W	208	-12.965	5 -18.384	52.877	1.00 32.22	W
25	MOTA	1228	OH2	W TAW	209	4.880	-15.352	25.292	1.00 74.89	W

	MOTA	1229	OH2 WAT W 210	-14.011 4.577	39.538 1.00 40.06	W
	MOTA	1230	OH2 WAT W 211	-18.207 -6.622	46.065 1.00 52.52	W
	MOTA	1231	OH2 WAT W 212	-1.942 -21.966	60.262 1.00 54.38	W
	MOTA	1232	OH2 WAT W 213	-10.025 2.738	39.161 1.00 89.20	W
5	MOTA	1233	OH2 WAT W 214	-7.536 3.097	34.665 1.00 66.61	W
	MOTA	1234	OH2 WAT W 215	-6.865 4.692	30.926 1.00 68.98	W
	MOTA	1235	OH2 WAT W 216	-5.056 6.596	40.134 1.00 47.28	W
	MOTA	1236	OH2 WAT W 217	-3.634 4.447	40.783 1.00 83.64	W
	MOTA	1237	OH2 WAT W 218	7.394 -11.367	25.281 1.00 57.42	W
10	MOTA	1238	OH2 WAT W 219	9.310 -21.158	25.421 1.00 59.90	W
	MOTA	1239	OH2 WAT W 220	10.366 -24.989	26.400 1.00 58.73	W
	MOTA	1240	OH2 WAT W 221	-4.606 3.348	26.800 1.00 65.51	W
	MOTA	1241	OH2 WAT W 222	-2.367 6.175	29.500 1.00 42.56	W
	MOTA	1242	OH2 WAT W 223	-4.942 6.474	32.978 1.00 55.44	W
15	MOTA	1243	OH2 WAT W 224	-20.607 -20.158	31.933 1.00 59.45	W
	MOTA	1244	OH2 WAT W 225	-25.839 -21.690	29.465 1.00 67.32	W
	MOTA	1245	OH2 WAT W 226	-27.537 -18.582	31.205 1.00 63.04	W
	MOTA	1246	OH2 WAT W 227	1.524 -5.767	50.296 1.00 37.51	W
	MOTA	1247	OH2 WAT W 228	-1.401 -5.768	53.755 1.00 58.16	W
20	MOTA	1248	OH2 WAT W 229	1.756 0.015	54.499 1.00 67.42	W
	MOTA	1249	OH2 WAT W 230	7.581 -7.200	53.652 1.00 51.29	W
	MOTA	1250	OH2 WAT W 231	10.564 -9.875	52.898 1.00 34.20	W
	MOTA	1251	OH2 WAT W 232	-12.228 8.044	49.309 1.00 43.27	W
	MOTA	1252	OH2 WAT W 233	3.892 -5.291	53.253 1.00 54.32	W
25	MOTA	1253	OH2 WAT W 234	-12.406 -27.193	54.213 1.00 58.17	W

	MOTA	1254	OH2	WAT W 235	-12.591 -26.874	57.492	1.00 59.02	W
	MOTA	1255	OH2	WAT W 236	-9.972 -27.101	55.248	1.00 64.22	W
	MOTA	1256	OH2	WAT W 237	-10.986 -26.023	59.916	1.00 85.99	W
	MOTA	1257	OH2	WAT W 238	-8.633 -24.722	60.499	1.00 65.65	W
5	MOTA	1258	OH2	WAT W 239	-7.408 -29.767	62.831	1.00104.46	W
	MOTA	1259	OH2	WAT W 240	-10.853 -30.151	64.764	1.00 64.63	W
	MOTA	1260	OH2	WAT W 241	-5.798 -30.088	64.947	1.00 59.64	W
	ATOM	1261	OH2	WAT W 242	-10.749 -26.762	64.393	1.00 42.38	W
	MOTA	1262	OH2	WAT W 243	-4.473 -23.155	64.989	1.00 62.66	W
10	MOTA	1263	OH2	WAT W 244	-7.538 -16.683	61.868	1.00 50.16	W
	ATOM	1264	OH2	WAT W 245	-10.230 -12.385	64.294	1.00 56.02	W
	ATOM	1265	OH2	WAT W 246	-12.542 -9.996	64.001	1.00 54.97	W
	ATOM	1266	OH2	WAT W 247	-3.345 -14.402	69.343	1.00 57.93	W
	MOTA	1267	OH2	WAT W 249	-3.709 -26.479	62.036	1.00 92.57	W
15	MOTA	1268	OH2	WAT W 250	-0.479 -31.295	63.228	1.00 47.82	W
	MOTA	1269	OH2	WAT W 251	-3.132 -28.329	67.027	1.00 81.69	W
	MOTA	1270	OH2	WAT W 252	1.056 -29.536	66.527	1.00 61.35	W
	MOTA	1271	OH2	WAT W 253	-1.744 -29.498	70.046	1.00 87.09	W
	MOTA	1272	OH2	WAT W 254	-3.689 -29.331	72.794	1.00 58.75	W
20	MOTA	1273	OH2	WAT W 255	-1.410 -27.800	75.675	1.00 97.58	W
	MOTA	1274	OH2	WAT W 256	-5.043 -29.537	76.343	1.00 64.90	W
	MOTA	1275	OH2	WAT W 257	-4.475 -32.406	78.585	1.00 63.31	W
	MOTA	1276	OH2	WAT W 258	-9.056 -33.080	76.962	1.00 69.69	W
	MOTA	1277	OH2	WAT W 259	-4.003 -31.163	82.151	1.00 71.55	W
25	MOTA	1278	OH2	WAT W 260	-5.860 -21.668	72.801	1.00 74.39	W

		MOTA	1279	OH2 WAT W 261	-2.868 -8.958	39.980	1.00 74.69	W
		MOTA	1280	OH2 WAT W 262	-4.140 -12.006	44.306	1.00 62.67	W
		MOTA	1281	OH2 WAT W 263	-3.803 -8.642	42.852	1.00 66.75	W
		MOTA	1282	OH2 WAT W 264	1.805 -10.509	35.249	1.00 59.42	W
	5	MOTA	1283	OH2 WAT W 265	-4.539 -24.842	50.726	1.00 36.51	W
		MOTA	1284	OH2 WAT W 266	-19.503 -1.261	38.826	1.00 69.86	W
		MOTA	1285	OH2 WAT W 267	12.469 -22.407	27.693	1.00 85.12	W